Anti-Newtonian Expansions, Hadamard States, and the Spatial Functional Renormalization Group

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The validity of general relativity almost up to the Big Bang entails that the Einstein equations themselves can be used to study the detailed structure of spacetime in the vicinity of the singularity. Within the cosmological paradigm of a Friedmann-Lemaître spacetime, where a description of physics in terms of quantum field theories (QFTs) on such a curved background is deemed to be valid, this mandates the existence of a pre-inflationary epoch following the Big Bang. Accepting this physically well-motivated scenario of a pre-inflationary phase as valid, this thesis aims to develop a customized theoretical framework for interacting scalar QFTs on generic Friedmann-Lemaître backgrounds. Importantly, such a framework cannot be in Euclidean signature (due to ill-definedness of a Wick rotation), nor should it be tailored towards de Sitter spacetime. Motivated by the subdominance of spatial gradients in the approach to the singularity, the major themes of this thesis are variants of spatial averaging and spatial gradient expansions in relation to the dependence on the underlying vacuum-like state.

The first of these themes is the Anti-Newtonian expansion in a spatially discretized setting. In this framework, the solution of a QFT decouples into two sub-problems: (i) the solution of the cosmological quantum mechanics; and (ii) the solution of the combinatorial problem that allows one to analytically control the terms of a "spatial hopping" expansion. The second theme is a novel manifestly Lorentzian formulation of the Functional Renormalization Group. The key differences of this formulation compared to the standard Euclidean setting are (i) it necessitates the incorporation of state-dependent aspects directly into the flow equation formalism; and (ii) the purely *spatial* mode modulation leads to an additional contribution to the renormalization of the Newton constant. In a full quantum gravity computation, the latter would quantitatively affect the interplay between the matter and gravity sectors. Within the asymptotic safety scenario, this interplay is believed to resolve

the triviality of scalar field theories. This has found phenomenological applications, which are however yet provisionary, because the infrared regime of the flow equation is neither well-posed nor controlled. This thesis prepares the tools to address this situation.

Table of Contents

List of Tables

List of Figures

1.0 Introduction

The generic occurrence of singularities in general relativity [48, 14, 35] is one of its most robust and remarkable features, signifying in a cosmological context the breakdown of the classical description of the evolution of Lorentzian spacetime at the Big Bang (or Big Crunch). However, the approach to this singularity in the past is hypothesized to ultimately be curtailed by the appearance of yet-to-be-understood quantum gravity effects. Following the Big Bang and the brief quantum gravity epoch, a description of physics in terms of quantum field theory on a classical spacetime described by the Einstein equations is presumed to be valid. The classical spacetime is thought to be well approximated by a (spatially flat) Friedmann-Lemaître spacetime whose expansion is driven by a homogeneous scalar field. In the modern cosmological paradigm, this evolution is hypothesized to have entered a quasi-de Sitter phase known as inflation shortly after the Big Bang, thereby solving the well-known *horizon, flatness, and monopole* problems [43, 64]. The linearized quantum fluctuations of the gravity-scalar system, treated within the framework of quantum field theory in curved spacetime, have notable consequences including seeding the inhomogeneities observed in the Cosmic Microwave Background [75]. More recently, non-linearities in the quantum fluctuations have been studied treating the quantum fields as evolving on a de Sitter background [11, 10].

The presumed validity of general relativity almost up to the Big Bang has further implications, namely it can be used to study the detailed structure of spacetime in the vicinity of the (spacelike) singularity. While the singularity theorems do not offer insight into spacetime in this regime, other techniques offer the following qualitative picture. In the approach to a spacelike singularity, spatial gradients become subleading compared to temporal ones. Further, the temporal approach to the singularity almost always displays one of two behaviors: either a rapid oscillatory (chaotic/mixmaster-type) approach or a power-like (quiescent) approach. Which of these two cases occurs depends on the matter content (and also on the number of spatial dimensions). The paradigmatic cases are a vacuum where mixmaster behavior is typical (as shown originally by Belinski-Khalatnikov-Lifshitz [12, 13]), and a

massless scalar field where a quiescent approach is generic as rigorously proven by Andersson and Rendall [2]. We draw on Penrose's intuition that the Big Bang should be viewed as being gravitationally simple in having low gravitational entropy (with respect to an appropriate mathematical notion thereof), which disfavors the chaotic approach. While the result of Andersson and Rendall only covers the free massless scalar, within the standard paradigm of a Friedmann-Lemaître spacetime driven by a scalar field with generic potential, stronger statements can be made. Mathematically rigorous arguments by Foster [38] as well as a data-driven analysis of Hergt et al. [50] show that a pre-inflationary phase with kinetic energy domination is preferred, i.e. the specific features of the scalar potential become irrelevant and the behavior resembles that of a Friedmann-Lemaître spacetime coupled to a (homogeneous) free massless field.

Accepting this well-motivated physical scenario of the existence of a pre-inflationary phase, during which the description of quantum field theories (QFT) on curved backgrounds is expected to be valid, in this thesis we strive to develop a customized theoretical framework for interacting scalar QFTs in this early kinetically dominated phase. Such a framework cannot be in Euclidean signature as the expanding spacetime generically prohibits a Wick rotation [6], nor should it be tailored towards de Sitter spacetime. Motivated by the subdominance of spatial gradients in the BKL scenario, we aim at developing variants of a spatial gradient expansion in the very early Universe. Moreover, since the classical potential underlying the inflationary paradigm is typically non-renormalizable, we wish to de-emphasize weak coupling and the specific form of the potential in the formalism. In renormalization group language, this suggests a Wilsonian approach, where all interaction monomials compatible with some prescribed symmetry are initially treated on the same footing. However, the standard approaches which are Wilsonian in spirit, namely lattice methods or the Functional Renormalization Group, strongly rely on Euclidean signature. In the present context, this necessitates a new adaptation of Wilsonian ideas to Friedmann-Lemaître spacetimes. The overall strategy to be pursued in this thesis is summarized in Figure 1, and we briefly comment on each of the elements here, and in more detail in the subsequent sections.

As displayed, the central idea is a form of spatial regularization or mode modulation. On the left side of the figure the spatial slices of the Friedmann-Lemaître spacetime are

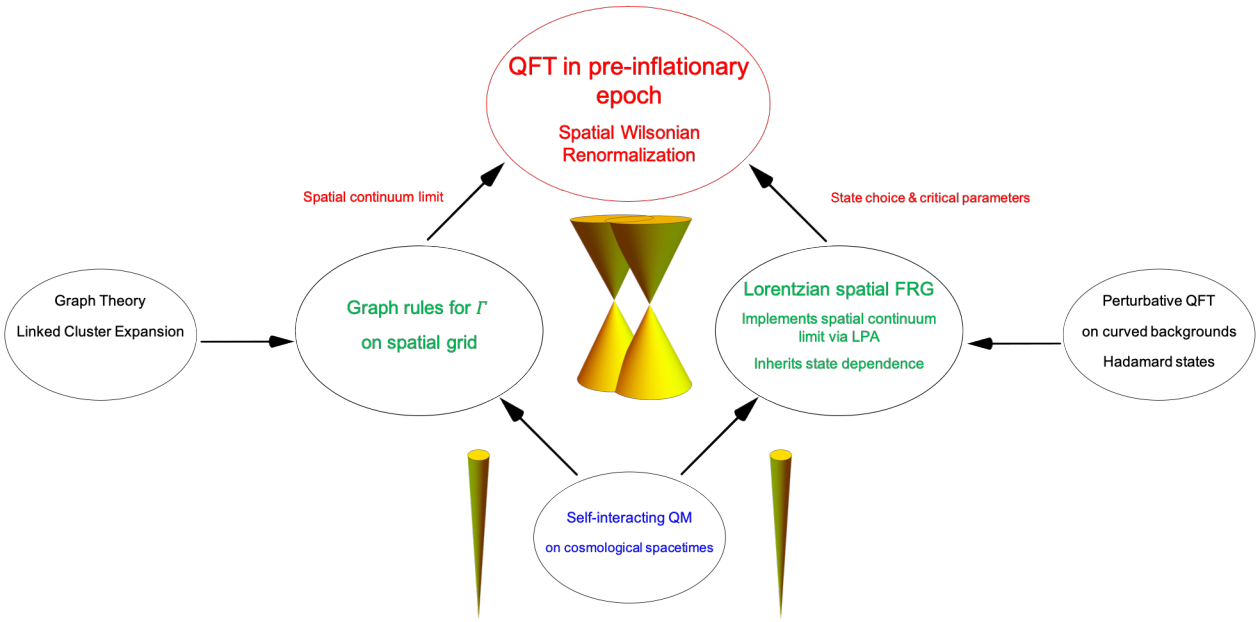


Figure 1: Summary of strategy for QFT in the early Universe.

discretized, while leaving time continuous (thereby avoiding discretization issues with the non-trivial temporal dynamics). This regularization lends itself to a novel expansion scheme in the spirit of the Linked Cluster Expansion (LCE) from statistical physics. Upon discretization, the QFT may be considered to be a collection of *spatially coupled* self-interacting quantum mechanical systems, one associated to each spatial lattice site. Perturbing in the spatial interaction generates an expansion about the *decoupled* quantum mechanical systems, the so-called Anti-Newtonian limit, where the lightcones shrink to lines. The solution of the (regularized) QFT under consideration then reduces to the evaluation of the *spatial* LCE or *spatial hopping expansion*, which may be efficiently developed utilizing graph theoretic methods as detailed in Chapters 2 and 3 of this thesis, together with a solution of the self-interacting quantum mechanics on the cosmological spacetime. Importantly, at no point is a Wick rotation necessary, and the systematics of the spatial hopping expansion are largely model independent thereby decoupling the details of the (typically non-renormalizable) potential from the spatial expansion.

The complementary approach on the right side of the figure is a novel *spatial* adaptation

of the Functional Renormalization Group (FRG) to Lorentzian spacetimes. The FRG is a work-horse for non-perturbative QFT, exclusively developed in Euclidean signature, and has found application in areas as diverse as solid-state physics, QCD, and quantum gravity (leading to the revival of the asymptotic safety scenario of Weinberg [100]). The key idea of the FRG approach (further detailed in Section 1.1.4) is to introduce an additional scale k through an infrared mode regulator kernel $\mathcal{R}_k$ that effectively gives slow-modes a mass of order k^2, while leaving the fast-modes untouched. This yields a family of k-dependent QFT functionals and equations for their k-flow, with modern approaches focussing on the Wetterich equation [103]

$$k\partial_k\Gamma_k[\phi] \;=\; \frac{\hbar}{2}\mathrm{Tr}\big\{k\partial_k\mathcal{R}_k[\Gamma_k^{(2)}+\mathcal{R}_k]^{-1}\big\} \tag{1}$$

for the flow of the scale dependent Legendre effective action Γ_k (also known as the "effective average action"). While the Euclidean nature of the approach is innocuous for solid-state physics or QCD as in principle Lorentzian QFT may be recovered through a Wick rotation (appealing to the Osterwalder-Schrader reconstruction theorem), in the context of quantum gravity or quantum field theory in curved spacetime it is known that a satisfactory general notion of a Wick rotation ceases to exist [6]. Related to the absence of a Wick rotation is the issue of vacuum state dependence in Lorentzian QFT, an aspect that is invisible in the Euclidean setting, but is pertinent to recent studies of the phenomenology associated to the non-Gaussian quantum gravity fixed point [32, 31]. Finally, the FRG may be used to obtain the critical parameters for the continuum limit of the hopping expansion (see Chapter 4), as well as offering an approach to the cosmological quantum mechanics.

In this thesis we reformulate the FRG equations manifestly in Lorentzian signature through the introduction of a *spatial mode modulation*, thereby avoiding the aforementioned issues with the problematic Wick rotation. The issues associated with vacuum state choice, studied rigorously in the context of perturbative QFT on curved backgrounds (see [61] and the references therein), may then be explored. In brief, in a Lorentzian setting the Hessian $\Gamma_k^{(2)}+\mathcal{R}_k$ in (1) is not elliptic and therefore lacks an unique inverse, reflecting the ambiguity in the choice of the two-point function for *free* QFTs on curved backgrounds. In non-maximally symmetric spacetimes in the latter context, one is faced with a large class of

physically admissible two-point functions, with the only requirement being that they satisfy the Hadamard property [60, 87]. The Hadamard property translates to a universal short distance singularity structure, but leaves the long range behavior unconstrained. In the context of the FRG equations this translates into a universal large k flow, while the choice of state will affect the flow to small k. Motivated by the schematic correspondence depicted in Figure 2,

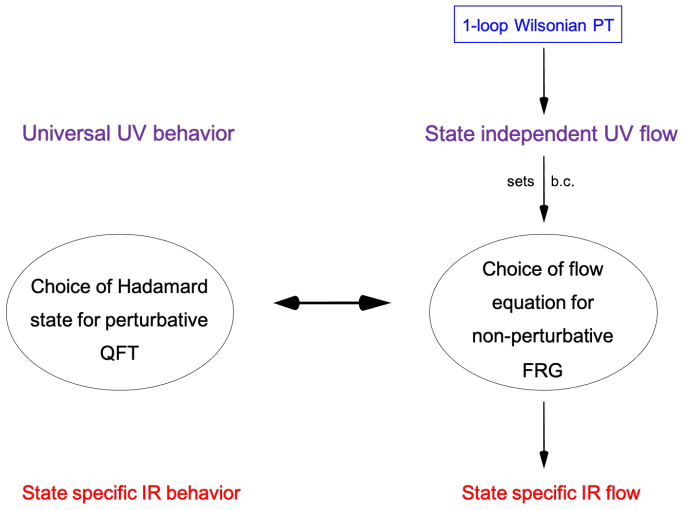


Figure 2: Correspondence between state choice in perturbative QFT and choice of flow equation for non-perturbative FRG.

in Chapter 5 we study a particular class of Hadamard states, known as States of Low Energy. Returning to the spatial FRG proper in Chapter 6, we study the RG flow of the one-loop effective action on Friedmann-Lemaître backgrounds, which sets the boundary conditions in the ultraviolet for the non-perturbative flow. We find that although the spatial regulator kernel breaks covariance, remarkably only covariant counter-terms are required for one-loop renormalization of a *generic* potential. Furthermore, the spatial averaging leads to an additional contribution to the renormalization of the Newton constant g_N, which in a full quantum gravity computation would quantitatively affect the interplay between the gravity and matter sectors.

The results presented in this thesis are based on the following publications:

Chapter	Article	arXiv
3	J.Math.Phys. 60 (2019) 1, 013504	arXiv:1812.06602
4	PoS LATTICE 2018 (2018) 249	arXiv:1812.02251
5	J.Math.Phys. 61 (2020) 103511	arXiv:2006.08685

Table 1: Publication list.

1.1 Background

In the following sections we present brief self-contained reviews of the elements entering Figure 1, and comment on how these relate to the original research in the subsequent chapters of this thesis.

1.1.1 Kinetic energy domination in scalar field cosmologies

Consider a spatially flat 1+d dimensional Friedmann-Lemaître spacetime with line element of the form

$$ds^2 = -N(t)^2\, dt^2 + a(t)^2 \delta_{ij} dx^i dx^i \,, \tag{2}$$

where the lapse $N(t)$ shall be treated as a degree of freedom so as to retain temporal reparameterization invariance[1]. The Friedmann-Lemaître spacetime is coupled to a spatially homogeneous field $\varphi(t)$ governed by a largely arbitrary potential $U(\varphi)$. Since the shift N^i has been set to zero in (2) the $(0,i)$, $i = 1,\ldots,d$, components of the field equations vanish identically. The remaining field equations read

$$d(d-1)(\partial_t a a^{-1})^2 - (\partial_t \varphi)^2 - 2N^2(U(\varphi)+\Lambda) = 0\,, \tag{3a}$$

$$a^{-(d-1)}\bar{N}\partial_t[a^{d-2}N^{-1}\partial_t a] - \frac{d-2}{2}(\partial_t a a^{-1})^2 + \frac{(\partial_t\varphi)^2}{2(d-1)} - \frac{N^2}{d-1}(U(\varphi)+\Lambda) = 0\,, \tag{3b}$$

[1]The lapse function $N(t)$ can be conveniently used to encode useful choices of time parameter such as cosmological time $N(t) = 1$, or conformal time $N(t) = a(t)$.

$$\partial_t(a^d N^{-1}\partial_t\varphi) + N a^d U'(\varphi) = 0\,, \tag{3c}$$

without gauge fixing. As indicated, we attribute the cosmological constant $\Lambda \geq 0$ to the gravitational sector, and normally assume that $U(\varphi)$ has no constant term. Using (3a) to eliminate $(\partial_t\varphi)^2$ from (3b), it can be rewritten in the more familiar form [2]

$$\frac{1}{N}\partial_t\Big(\frac{a^d}{N}\frac{\partial_t a}{a}\Big) - \frac{2}{d-1}a^d[U(\varphi)+\Lambda] = 0\,. \tag{4}$$

The dependence on the scalar field may be reexpressed through the energy density ρ and the pressure $\mathcal{P}$

$$\begin{aligned} \rho &= \frac{1}{2}N^{-2}(\partial_t\varphi)^2 + U(\varphi)\,, \\ \mathcal{P} &= \frac{1}{2}N^{-2}(\partial_t\varphi)^2 - U(\varphi)\,, \end{aligned} \tag{5}$$

which parameterize the nonzero components of the energy momentum tensor via $T_{00} = \rho, T_{ij} = \delta_{ij}\mathcal{P}$. We shall assume the weak energy condition throughout, $\rho \geq 0, \rho+\mathcal{P} \geq 0$. Due to (5), it is clear that non-negative potentials are sufficient for the weak energy condition to hold. Moreover, in Friedmann-Lemaître spacetimes the Weyl tensor vanishes identically and the singularity is signaled by the divergence of

$$[R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R(g)][R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R(g)] = [T^{\mu\nu} - g^{\mu\nu}\Lambda][T_{\mu\nu} - g_{\mu\nu}\Lambda] = (\rho+\Lambda)^2 + d(\mathcal{P}-\Lambda)^2\,, \tag{6}$$

while the Ricci scalar may stay finite. Hence at least one of $\rho+\Lambda, \mathcal{P}-\Lambda$ must diverge at the singularity, $t \to t_{\rm sing}$.

Since we consider strictly monotonically expanding spacetimes, $N^{-1}\partial_t a > 0$, the Hubble distance $d_H(t) := a(t)/[N^{-1}\partial_t a] > 0$ then sets an intrinsic length scale. It is instructive to rewrite the equations (3) in terms of (5) and d_H,

$$\frac{1}{d_H^2} = \frac{2}{d(d-1)}(\rho+\Lambda)\,, \tag{7a}$$

$$\frac{N^{-1}\partial_t d_H}{d_H^2} = \frac{1}{d-1}(\rho+\mathcal{P})\,, \tag{7b}$$

$$N^{-1}\partial_t\rho = -\frac{d}{d_H}(\rho+\mathcal{P})\,, \tag{7c}$$

[2] The constraint (3a) is by construction preserved under the evolution (3c), (4).

again without gauge fixing. On account of the second equation the Hubble distance is nondecreasing for matter obeying the weak energy condition. Moreover

$$\text{deceleration: } 1 \leq N^{-1}\partial_t d_H < \infty\,, \quad \text{acceleration: } N^{-1}\partial_t d_H < 1\,, \tag{8}$$

where the shifted strong energy condition, $(d-2)(\rho+\Lambda) + d(\mathcal{P}-\Lambda) \geq 0$, $d \geq 3$, implies deceleration. As indicated, we exclude a diverging $N^{-1}\partial_t d_H$. Using (7a), (7b) in (6) one finds for the right hand side $d(d-1)[1/2 + N^{-1}\partial_t d_H]/d_H^2$. Hence $d_H \to 0$ for $t \to t_{\text{sing}}$. This motivates the following definition of a *pre-inflationary* Friedmann-Lemaître spacetime:

Definition 1.1.1.

A spatially flat FL geometry (2) is called *pre-inflationary* if $a, N : I \to \mathbb{R}_+$, $I = [t_{\text{sing}}, t_f]$, $t_{\text{sing}} \in [-\infty, 0]$, $t_f \in (t_{\text{sing}}, \infty]$, such that $1 \leq N^{-1}\partial_t d_H < \infty$ for $t \in I$ with $a(t), d_H(t) \to 0^+$ for $t \to t_{\text{sing}}$.

Finally, remarkably general statements about the early time asymptotics of spatially flat FL cosmologies driven by a scalar field can be made, from which follows the existence of a pre-inflationary period. We consider smooth potentials of the following form

$$\begin{aligned} &U(\varphi) \geq 0\,, \quad U(\varphi) > 0\,, \quad \pm\varphi > \varphi_\pm > 0 \ \text{ for some } \varphi_\pm > 0\,, \\ &\lim_{\varphi\to\pm\infty} \frac{U'(\varphi)}{U(\varphi)} - \epsilon_\pm = 0\,, \quad \text{for some } \ -\infty < \epsilon_\pm < \sqrt{\frac{4d}{d-1}}\,. \end{aligned} \tag{9}$$

As seen before $U(\varphi) \geq 0$ is a sufficient condition for the weak energy condition to hold, the additional proviso eliminates potentials of compact support. The second condition restricts the rate of growth of the potential at infinity to be less than $\exp\{\sqrt{4d/(d-1)}|\varphi|\}$. This class of potentials is very broad: it includes positive polynomials, linear combinations of exponentials (subject to the growth conditions), and all logarithmic modifications thereof. Examples of the latter are

$$U(\varphi) = U_0\, \varphi^n (\log\varphi)^m e^{-\gamma\varphi/(\log\varphi)^l}\,, \quad U_0, \gamma, l > 0\,, \ \ m, n \in \mathbb{R}\,, \tag{10}$$

for $\varphi > \varphi_+$, and similarly for negative φ. Virtually all explicit potentials discussed in the literature on 'single field inflation' fall into the above class. In addition to (9) a technical regularity assumption ("well behaved at infinity") is needed on how infinity is approached.

Under these conditions S. Foster [38] showed (in $d = 3$) the following important

Result: Let $U(\varphi)$ be a potential of the form (9) well behaved at infinity and consider the spatially flat FL equations (3) in $N(t) = 1$ gauge. Then almost all solutions have an initial singularity at $t=0$ which they approach in the following universal manner:

$$\begin{aligned} \frac{\partial_t a}{a} &= \frac{1}{d\,t} + O(\epsilon_U^{\pm}(t))\,, \\ \varphi(t) &= \pm\sqrt{\frac{d-1}{d}}\ln t/t_i + O(t\epsilon_U^{\pm}(t))\,, \\ \partial_t\varphi &= \pm\sqrt{\frac{d-1}{d}}\frac{1}{t} + O(\epsilon_U^{\pm}(t))\,, \end{aligned} \tag{11}$$

where $\epsilon_U^{\pm}(t) = t\,U(\pm\sqrt{(d-1)/d}\ln t)$.

The leading asymptotics is that of a 'stiff fluid', $a(t) \propto t^{1/d}$. In other words, the influence of the potential $U(\varphi)$ on the scalar field cosmology is wiped out near the singularity and the approach to it is the same as if matter consisted of a free massless field! This result provides a mathematical backing for the existence of a 'preinflationary phase' where kinetic energy dominates over potential energy. Moreover, it is arrived at within the same classical general relativistic framework that underlies inflationary spacetimes.

1.1.2 Perturbative QFT in curved spacetime: the Hadamard Property

Perturbative quantum field theory begins with the quantization of the linear free field, subsequently followed by the introduction of non-linearities. In this section we briefly review the quantization of the Klein-Gordon field, referring to the standard texts [99, 40, 15, 81] for further details. We begin with a quick summary of the Minkowski spacetime version,

$$[-\eta^{\mu\nu}\partial_\mu\partial_\nu + m^2]\varphi \;=\; 0 \tag{12}$$

tailored towards identifying the aspects that do or do not carry over to generic globally hyperbolic manifolds. Following [40], we shall begin with the "particle" viewpoint and subsequently "discover" the field. The translational invariance of Minkowski spacetime entails the existence of the spacetime Fourier transform $f^\wedge(p) \;=\; \int d^4y\, e^{-ipy} f(y)$, such that the

solutions of (12) in momentum space live on the upper and lower mass-shells

$$X_m^{\pm} := \{p \in \mathbb{R}^4 \,|\, p^2 = m^2\,,\; 0 \lessgtr p^0\}\,. \tag{13}$$

Each mass-shell is an embedded submanifold of $(\mathbb{R}^4, \eta)$, inheriting the hyperbolic metric from the Minkowski metric η via pullback, and thereby the associated Lorentz invariant volume form. Regarding the quantized Klein-Gordon theory as describing relativistic particles of mass m, one applies the "physical" requirement that their energy be positive and hence defines the one-particle Hilbert space as *the space of square integrable functions on the positive mass-shell*, $\mathcal{H} = L^2(X_m^+)$, with Lorentz invariant inner product

$$\langle f, g\rangle = \int_{\mathbb{R}^3} \frac{d^3p}{(2\pi)^3\omega_p} f(p)^* g(p)\,, \quad \omega_p := \sqrt{p^2 + m^2} \quad \forall\, p \in \mathbb{R}^3\,. \tag{14}$$

Performing the inverse Fourier transform to position space, $f^\vee(t,x) = \int_{\mathbb{R}^3} \frac{d^3p}{(2\pi)^3\omega_p} e^{-i\omega_p t + ipx} f(p)$, one readily sees that the position space representation of $\mathcal{H}$ is the subspace $\mathcal{S}^+$ of the solution space $\mathcal{S}$ of the Klein-Gordon equation (12) consisting of purely positive frequency solutions. Moreover, when restricted to $\mathcal{S}^+$ the Klein-Gordon symplectic form Ω_{KG} is actually an inner product, specifically for $f, g \in L^2(X_m^+)$

$$\langle f, g\rangle = \frac{i}{2}\Omega_{KG}(f^\vee, g^\vee) := \frac{i}{2}\int_{t=0} d^3x \big[f^{\vee *}\partial_t g^\vee - \partial_t f^{\vee *} g^\vee\big]\,. \tag{15}$$

It is precisely this choice of subspace $\mathcal{S}^+$ of the (complexified) solution space $\mathcal{S}$ of the Klein-Gordon equation, on which Ω_{KG} restricts to an inner product, that entails the non-uniqueness of the vacuum on generic spacetimes [99], a point to which we return in a moment. The standard QFT construction is then completed by defining the multiparticle Bosonic Fock space $\mathscr{F} := \overline{\mathbb{C} \oplus \mathcal{H} \oplus \mathcal{H}^{\odot 2} \oplus \dots}$ as the direct sum of symmetric tensor products[3], with the Fock vacuum $|0\rangle = (1, 0, 0, \dots)$ in direct sum notation. Next, one introduces the creation and annihilation operator (-valued distributions) $\mathbf{a}(p)^*, \mathbf{a}(p)$ such that

$$[\mathbf{a}(p), \mathbf{a}(p')^*] = (2\pi)^3\delta^{(3)}(p - p')\,, \quad \mathbf{a}(p)|0\rangle = 0 \quad \forall\, p, \tag{16}$$

[3]The closure being taken with respect to the inner-product induced by that on $\mathcal{H}$.

and subsequently the field operator

$$\hat{\varphi}(t,x) = \int \frac{d^3p}{(2\pi)^3} \Big\{ \frac{e^{-i\omega_p t + ipx}}{\sqrt{2\omega_p}} \mathbf{a}(p) + \frac{e^{i\omega_p t - ipx}}{\sqrt{2\omega_p}} \mathbf{a}(p)^* \Big\} . \tag{17}$$

Being a linear combination of *both* creation and annihilation operators it is readily verified that

$$[\hat{\varphi}(t,x), \hat{\varphi}(t',x')] \;=\; i\Delta(t,x;t',x') \tag{18}$$

where Δ is the Pauli-Jordan function. The vanishing of $\Delta(y,y')$ for spacelike separated coordinates thus entails the desired commutativity of field operators for spacelike separation. Furthermore, this construction yields the standard unitary representation of the Poincaré group for scalar fields, and the usual development of canonical perturbative QFT via normal ordering and Wick products follows straightforwardly from this point.

While the above construction apparently makes heavy use of the spacetime Fourier transform and associated particle interpretation (neither of which is generally available in curved spacetime) these are not strictly necessary for quantization of the linear theory as stressed by Wald [99]. From this perspective, the essential "physical" input is the identification of a subspace $\mathcal{S}'$ of the (complexified) solution space $\mathcal{S}$ of the Klein-Gordon equation (12) such that the symplectic form Ω_{KG} restricted to $\mathcal{S}'$ is a positive-definite inner product. This subspace $\mathcal{S}'$ together with the inner product then serves as the one-particle Hilbert space underlying the Fock space construction and definition of the field operators. Thus, the choice of $\mathcal{S}'$ is equivalent to the *choice of vacuum state* $|0\rangle$. On Minkowski spacetime, or indeed any stationary spacetimes admitting a global timelike Killing vector field, the canonical identification of $\mathcal{S}'$ as the subspace of *positive frequency solutions* yields the standard construction [3, 59]. For the Friedmann-Lemaître spacetimes that are the focus of this thesis, such an identification is not generically possible, rendering the choice of vacuum state inherently ambiguous.

In order to disentangle the algebraic properties of the field operators from the specifics of a Hilbert space representation (which are generically not unitarily equivalent due to the failure of the Stone-von Neumann theorem in the infinite dimensional setting), modern formulations of QFT on curved backgrounds take the algebraic approach [61]. Briefly, on a globally

hyperbolic manifold (M, g), the Cauchy problem for the Klein-Gordon equation is well-posed, hence so is the phase-space formulation. Canonical quantization allows a transition to the algebra of observables $\mathcal{A}(M)$ generated by smeared field operators $\varphi(f)$, $f \in C_c^\infty(M)$. The quantization procedure of replacing Poisson brackets with commutators, $\{\cdot,\cdot\} \mapsto i[\cdot,\cdot]$ then yields the commutation relation

$$[\varphi(f), \varphi(g)] \;=\; i\Delta(f,g)\,, \tag{19}$$

where Δ is the commutator function, determined entirely by classical data.

A vacuum-representation of the field algebra $\mathcal{A}(M)$ on a Hilbert space arises through the selection of a "homogeneous pure quasi-free" state ω, which is a positive linear functional over the field algebra $\mathcal{A}(M)$, followed by the Gelfand-Naimark-Segal (GNS) construction. Here "pure" means that ω cannot be written as a convex combination of other states, while "quasi-free" entails that all odd n-point functions vanish while the even n-point functions can be expressed in terms of the two-point function $W(y, y')$ via Wick's theorem. The GNS construction selects a unique cyclic element Ω_ω in the reconstructed state space $\mathscr{F}_\omega$ such that the n-point functions are realized as expectation values of (the GNS reconstructed) field operators, e.g. $W(y, y') = (\Omega_\omega, \varphi(y)\varphi(y')\Omega_\omega)$. Specializing to a $1 + d$ dimensional spatially flat Friedmann-Lemaître spacetime for concreteness, the GNS vector Ω_ω turns out to correspond to a Fock vacuum $|0_\omega\rangle$, annihilated by annihilation operators defined by a mode expansion of the Heisenberg field operator

$$\begin{aligned} \varphi(t,x) &= \int \frac{d^d p}{(2\pi)^d} \big[T_p(t)\mathbf{a}_T(p)e^{ipx} + T_p(t)^*\mathbf{a}_T^*(p)e^{-ipx}\big]\,, \\ \big[\mathbf{a}_T(p), \mathbf{a}_T^*(p')\big] &= (2\pi)^d\delta(p-p')\,, \quad \mathbf{a}_T(p)|0_\omega\rangle = 0\,, \end{aligned} \tag{20}$$

where $T_p(t)$ is a Wronskian normalized complex solution of the spatially Fourier transformed Klein-Gordon equation (12). Then the two-point function may be realized as

$$W(t,x;t',x') = \langle 0_\omega|\varphi(t,x)\varphi(t',x')|0_\omega\rangle = \int \frac{dp}{(2\pi)^d}\, T_p(t)\, T_p(t')^*\, e^{ip(x-x')}\,. \tag{21}$$

One sees that modulo phase choices a "homogeneous pure quasifree" state is characterized by a choice of Wronskian normalized solution $T_p(t)$ of the wave equation or, equivalently,

by a choice of Fock vacuum $|0_\omega\rangle$ via (20), making manifest the ambiguity in state choice. Due to this equivalence we shall refer to the Fock vacuum as $|0_T\rangle$ in Chapter 5 to explicitly denote the dependence on $T_p(t)$.

However, not all states ω are physically admissible as one wishes to define quadratic and higher powers of the field operators in order to e.g. study the stress-energy tensor or develop perturbation theory. As usual, the naive definition of objects like "$\varphi(x)^2$" is obstructed by the distributional nature of $\varphi(x)$ and the associated short distance singularities. A general consensus is that the free state ω on which perturbation theory is based should be a **Hadamard state**, with the Hadamard property being by-and-large necessary and sufficient for the existence of Wick powers of arbitrary order and hence for the perturbative series to be termwise well-defined at any order, see [61, 36] for recent accounts. Physically, the Hadamard property can be interpreted as an instance of the equivalence principle, i.e. at small geodesic separation the singularity structure of a two-point function $W(y, y')$ should be akin to that in Minkowski spacetime. The original rigorous formulation of the Hadamard condition given by Kay and Wald [60] states that for sufficiently close spacetime coordinates y, y' (specifically lying in a convex normal neighborhood) the two-point function W matches the *Hadamard parametrix* $H_{\epsilon,d}$ up to a symmetric smooth part $\widetilde{W}$. Specifically,

$$\begin{aligned} W(y,y') &= N_d[H_{\epsilon,d}(y,y') + \widetilde{W}(y,y')]\,, \quad N_d = \frac{\Gamma(\frac{d-1}{2})}{2(2\pi)^{(d+1)/2}}\,, \\ H_{\epsilon,d}(y,y') &= \begin{cases} \dfrac{U(y,y')}{\sigma_\epsilon(y,y')^{\frac{d-1}{2}}} + V(y,y')\ln\mu^2\sigma_\epsilon(y,y') & d \text{ odd} \\ \dfrac{U(y,y')}{\sigma_\epsilon(y,y')^{\frac{d-1}{2}}} & d \text{ even} \end{cases}, \\ \sigma_\epsilon(y,y') &:= \sigma(y,y') + i\epsilon[t(y) - t(y')] + O(\epsilon^2)\,, \end{aligned} \tag{22}$$

for small $\epsilon > 0$, with $\mu > 0$ a mass parameter making the argument of the logarithm dimensionless. The Synge function $\sigma(y, y')$ is defined as one half of the square of the geodesic distance between the points with coordinates y, y'. Further, U and V are smooth symmetric local biscalar functions, determined entirely by the local geometry, and may hence be regarded as "universal", while the smooth piece $\widetilde{W}$ encodes the ambiguity of state selection. The bi-

scalars U and V are generally not exactly computable, but may be accessed through a double power series in σ_ϵ and its gradients, see e.g. [27]. In Friedmann-Lemaître spacetimes a far simpler characterization of the Hadamard property is available through the Gelfand-Dickey expansion presented in Section 5.4. Finally, although the formulation of the Hadamard condition in (22) explicitly captures the short distance similarity to Minkowski spacetime, it does not lend itself to analytic techniques. Thus contemporary formulations of the Hadamard condition use the equivalent microlocal definition given by Radzikowski [87] in terms of the wavefront set of the two-point function. We shall review this definition and the associated microlocal notions in Section 5.6.

On the other hand, Hadamard states are surprisingly difficult to construct concretely [24, 56, 17] even for background spacetimes with some degree of symmetry (other than maximal). The well-known adiabatic iteration [81] has certain characteristics necessary for the Hadamard property built in, but is not convergent and cannot be fruitfully extended to small spatial momenta. The iteration can, however, serve as a conduit to establish the existence of states locally indistinguishable from Hadamard states [56]. On Friedmann-Lemaître spacetimes, a construction of exact Hadamard states has become available only relatively recently [80]. These "States of Low Energy" (SLE) arise by minimizing the Hamiltonian's expectation value *after* averaging with a temporal window function f. The temporal averaging is crucial and avoids the pathologies [41] of the earlier instantaneous diagonalization procedure. In Chapter 5 we prove that the SLE have a number of bonus properties that make them mathematically even more appealing and which also render them good candidates for vacuum-like states in a pre-inflationary period. Specifically, we show that for a given temporal averaging function f:

(a) The SLE two-point function $W[S]$ based on a fiducial solution S of the spatially Fourier transformed Klein-Gordon equation (193) is a Bogoliubov invariant, $W[aS + bS^*] = W[S]$, with $a, b \in \mathbb{C}$, $|a|^2 - |b|^2 = 1$. Hence $W[S]$ is independent of the choice of fiducial solution S.

(b) The minimization over Bogoliubov parameters relative to a given S can be replaced by a minimization over initial data, without reference to any fiducial solution. The resulting expression for the SLE solution $T[\Delta]$ is fully determined by the (Bogoliubov invariant

and state independent) commutator function Δ, making manifest the uniqueness of the SLE. The minimization over initial data has a natural interpretation in the Schrödinger picture.

(c) The SLE solution admits a *convergent* series expansion in powers of the (modulus of the) spatial momentum, both for massive and for massless theories.

(d) In the massless case the leading infrared behavior is Minkowski-like for *all* cosmological scale factors. This provides a new cure for the long standing infrared divergences in Friedmann-Lemaître backgrounds with accelerated expansion [37].

(e) The modulus square of an SLE solution admits an asymptotic expansion in inverse odd powers of the (modulus of the) spatial momentum, which is *independent of the window function* f. The coefficients of the expansion are *local*, recursively computable, and generalize the heat kernel coefficients. The asymptotics of the phase is governed by single integrals of the same coefficients. This short cuts the detour via the adiabatic expansion.

Finally, while the energy minimization property of the SLE is physically appealing, we show that on a mathematical level the key aspect of the construction is not the minimization but rather the temporal averaging in Section 5.6. Specifically we construct a one parameter deformation of the SLE, dubbed "Generalized States of Low Energy" (GSLE) and prove that they are exact Hadamard states.

1.1.3 The hopping expansion

Lattice systems are ubiquitous in statistical physics, and also provide a regularization framework for (Euclidean) quantum field theories. We consider a bosonic theory defined on a D-dimensional hypercubic lattice Λ with spacing a, whose complete (statistical) information is encoded in the partition function

$$Z[J] := \int \prod_{x\in\Lambda} d\varphi_x \, e^{-S[\varphi]+\varphi\cdot J} \,. \tag{23}$$

and its related functionals. However, an exact evaluation of (23) is feasible only in extremely special circumstances, necessitating the use of approximation schemes, such as series (or

perturbative) expansions around an exactly soluble situation, to glean the properties of the system. There are typically two limiting theories associated with (23) where an exact computation of $Z[J]/Z[0]$ is feasible. The first is the familiar *Gaussian* theory where $S[\varphi]$ is a quadratic functional of φ; perturbation theory about this limit is a powerful tool, but with the drawback that this expansion is only asymptotic (with zero radius of convergence).

The lattice formulation, however, allows for another exactly soluble limit – the single site theory. This arises from expressing (23) schematically as

$$Z[J] \;=\; \int \prod_{x\in\Lambda} d\varphi_x \exp\Big\{ -S_{\substack{\text{single}\\ \text{site}}}[\varphi] - S_{\text{linking}}[\varphi] \Big\} = \int \prod_{x\in\Lambda} d\mu(\varphi_x)\, e^{-S_{\text{linking}}[\varphi]}\,, \qquad (24)$$

where the single-site term consists only of terms living at a single lattice point x, while the linking term consists of terms linking (potentially) distinct lattice points. The single site theory (with no linking) can be computed exactly as a product of ordinary integrals

$$Z_{\substack{\text{single}\\ \text{site}}}[J] \;=\; \int \prod_{x\in\Lambda} d\mu(\varphi_x) = \Big[\int d\mu(\varphi) \Big]^{|\Lambda|}\,, \qquad (25)$$

and perturbation theory in the "number of neighbor links" can be developed about this limiting case. When computing $\ln Z$, the expansion can be efficiently represented as a sum over *connected graphs*, hence the name "linked cluster expansion" (LCE). Alternatively the expansion is known as the "high temperature expansion" from the Ising model, or the "hopping expansion" (so called because the excitations seemingly "hop" between lattice sites).

For illustrative purposes, we shall focus on a particular model, namely scalar φ^4-theory on a D-dimensional hypercubic lattice $\Lambda = (a\mathbb{Z})^D$, with action

$$S[\varphi_0] \;=\; \sum_{x\in\Lambda} a^D \Big\{ -\tfrac{1}{2}\varphi_0 \nabla^2 \varphi_0 + \tfrac{1}{2} m_0^2 \varphi_0^2 + \tfrac{1}{4!} g_0 \varphi_0^4 \Big\}\,. \qquad (26)$$

Here φ_0 is the dimensionful bare field, and ∇^2 is the lattice Laplacian, which may be expressed terms of the hopping matrix ℓ (which links only nearest neighbors) as $-\nabla^2 = 2Da^{-2}\mathbf{1} - 2a^{-2}\ell$. As usual, in order to set up the hopping expansion proper one rewrites (26) in terms of dimensionless variables, viz

$$S[\varphi] \;=\; \sum_x s(\varphi_x) - \frac{\kappa}{2} \sum_{x,y} \varphi_x \ell_{xy} \varphi_y\,,$$

$$s(\varphi) \;=\; \varphi^2 + \lambda(\varphi^2-1)^2 - \lambda\,, \quad \ell_{xy} = \sum_i (\delta_{x,y+a\hat{e}_i} + \delta_{x,y-a\hat{e}_i})\,, \tag{27}$$

$$\frac{g_0}{a^{D-4}} \;=\; \frac{24\lambda}{\kappa^2}\,, \quad a^2 m_0^2 = \frac{2}{\kappa}(1-2\lambda) - 2D\,, \quad a^{\frac{D-2}{2}}\varphi_0(x) = \sqrt{\kappa}\,\varphi_x\,.$$

The partition function $Z_\kappa[J]$ then depends parametrically on κ, λ and is exactly computable via (25) for $\kappa = 0$. The hopping expansion is an expansion in powers of κ. Both the generating functional of *connected* correlation functions $W_\kappa[J]$, or its Legendre transform $\Gamma_\kappa[\phi]$, can in principle be expanded to any desired order in κ. As detailed in Chapters 2 and 3, these functionals satisfy κ-flow equations which can be used to recursively compute the hopping expansion. Direct iteration of these recursions is however unwieldy, but they can be solved using graph theoretic methods; the graph rules for W_κ are presented in [105], while those for Γ_κ are proven in Chapter 3.

Among the quantities computable via the hopping expansion are the generalized susceptibilities

$$\begin{aligned} \chi_2 \;&:=\; \sum_{x\in\Lambda} \langle \varphi_x \varphi_0 \rangle^{\mathrm{c}}\,, \quad \mu_2 := \sum_{x\in\Lambda} x^2 \langle \varphi_x \varphi_0 \rangle^{\mathrm{c}}\,, \quad x^2 = \sum_i x_i^2\,, \\ \chi_4 \;&:=\; \sum_{x,y,z\in\Lambda} \langle \varphi_x \varphi_y \varphi_z \varphi_0 \rangle^{\mathrm{c}}\,, \end{aligned} \tag{28}$$

where as usual

$$\langle \varphi_{x_1} \dots \varphi_{x_n} \rangle^c := \left. \frac{\delta^n W[J]}{\delta J_{x_1} \dots J_{x_n}} \right|_{J=0}\,. \tag{29}$$

The κ series for χ_2, μ_2, χ_4 can be shown to be convergent on a finite lattice and to have finite radius of convergence $\kappa < \kappa_c$ in the $\varphi \mapsto -\varphi$ symmetric phase even for infinite lattice volume. In the latter case the pole in the expansion lies on the positive real axis [73], indicating a physical singularity or phase transition. This second order phase transition is characterized by a diverging correlation length ξ, wherein the continuum limit of the lattice QFT may be defined.

The radius of convergence is typically determined from the χ_2 series via the ratio criterion: $\kappa_c = \lim_{n\to\infty} |\chi_{2,n}/\chi_{2,n+1}|$ where $\chi_2 = \sum_{n\geq 0} \kappa^n \chi_{2,n}$. On the other hand from the scaling

hypothesis one has $\chi_2 \propto (1-\kappa/\kappa_c)^{-\gamma}$, for $\kappa \to \kappa_c^-$. From its Taylor expansion one finds

$$\frac{\chi_{2,n}}{\chi_{2,n-1}} = \frac{1}{\kappa_c}\Big(1 + \frac{\gamma-1}{n} + o(n^{-1})\Big)\,, \quad \text{for } \; n \to \infty\,. \tag{30}$$

In principle κ_c and γ can be determined from a fit of the ratios once the κ-series for χ_2 has been computed to sufficiently large order. Technically it is advantageous to express χ_2, μ_2 in terms of a 1-particle irreducible χ_2^{1PI}, see [73]. The renormalized mass m_R in lattice units, the wavefunction renormalization constant Z_R, and the renormalized coupling g_R can be expressed in terms of the above susceptibilities

$$m_R^2 = 2D\,\frac{\chi_2}{\mu_2}\,, \quad Z_R = \chi_2\, m_R^2\,, \quad g_R = 4D^2\,\frac{\chi_4}{\mu_2^2}\,. \tag{31}$$

We omit the derivation and merely note the defining relations in terms of the moments of the effective action Γ in momentum space: $\Gamma^{(2)}(p,-p) = -Z_R^{-1}[m_R^2 + p^2 + O(p^4)]$ defines Z_R, m_R as $p = (p_0 = 0, \vec{p})$, with $\vec{p} \to 0$. Similarly $\Gamma^{(4)}(0,0,0,0) = -g_R/Z_R^2$ defines g_R. Finally, the correlation length ξ is defined as $1/m_R$ and equals the inverse pole mass $1/m_P$ up to higher orders in m_P. By definition ξ diverges with the exponent ν at a second order phase transition so that

$$\xi^2 = \frac{1}{m_R^2} \propto \Big(1 - \frac{\kappa}{\kappa_c}\Big)^{-2\nu}\,, \quad \kappa \to \kappa_c^-\,. \tag{32}$$

In a quantum field theory context, the hopping expansion was famously employed by Lüscher-Weisz in their (de-facto quantitative) proof of the triviality of Euclidean lattice φ_4^4-theory [69], where the critical parameters of the theory (λ, κ_c) were computed by pushing the hopping expansion to high orders. Moreover, the hopping series was used for $\kappa = 0.95\kappa_c$ to compute m_R^2, g_R, and these were subsequently evolved to the continuum limit under the Callan-Symanzik equation. It should be noted, however, that the determination of κ_c and the critical exponents from the radius of convergence of the hopping expansion requires considerable effort: the classification of graphs, the computer generation of billions of them, as well as estimates on the extrapolation of the expansion to infinite order. In Chapter 4 we present an alternative (and significantly simpler) computation of the critical lines of Euclidean ϕ_3^4- and ϕ_4^4-theory using the Local Potential Ansatz (LPA) truncation of the Functional Renormalization Group.

Finally, we end this short review of the hopping expansion by noting that the Anti-Newtonian expansion introduced in Chapter 2 amounts to a spatial variant of a LCE. The evaluation of some correlation function is reduced to a combinatorial and a QM problem. While the adaptation to a functional setting and the Friedmann-Lemaître spacetimes is not immediate, the functional analytical raison d'être of the benign convergence properties of (spatial) hopping expansion clearly remains valid: the perturbation (quadratic in the field) is Kato bounded [58, 92] by the unperturbed Hamiltonian (more than quadratic in the field). Irrespective of technical details one may reasonably expect the spatial LCE to have improved convergence properties compared to perturbation theory.

1.1.4 The Functional Renormalization Group

The Functional Renormalization Group (FRG) is a widely used reformulation of quantum field theory in the spirit of the Wilsonian Renormalization Group. Favored for its ability to go beyond the weak-coupling expansions of standard perturbation theory, it has found application in areas diverse as solid-state physics, particle physics, and quantum gravity. The central objects of study in the FRG are one-parameter families of QFT functionals, whose behavior is captured in the form of integro-differential flow equations. Thus, the usual QFT problem of evaluating the functional integral for some bare action (33) is replaced with integrating these flow equations. For a systematic exposition of the details of this technique and its applications we refer to [63, 104, 82, 30, 74, 102], focussing here instead on a schematic overview of the FRG as it pertains to the problems addressed in this thesis.

In order to construct the FRG equations and explicate the relevant issues, we focus on a single scalar field χ on a D dimensional Riemannian manifold $(\mathcal{M}, g)$. One begins with the source-dependent partition function $Z_\Lambda[J]$ (or generating functional $W_\Lambda[J] = \ln Z_\Lambda[J]$)

$$Z_\Lambda[J] \equiv e^{W_\Lambda[J]} := \int \mathcal{D}\chi_\Lambda e^{-S_\Lambda[\chi]+J\cdot\chi}\,, \tag{33}$$

with momentum cutoff Λ as a UV regularization, and "$\cdot$" denoting integration with respect to the Riemannian volume form $\int_{\mathcal{M}} \sqrt{g}$. In the Wilsonian renormalization group proper [83] the functional integral is performed piecemeal, integrating out fast-modes and retaining

slow-modes (typically distinguished by the spectral value of the manifold Laplacian ∇^2), while keeping the low energy physics unchanged. This "coarse graining" operation generates a flow in the Wilsonian actions $S_{b\Lambda}$ with $b \in (0,1)$, which are in general structurally different from the original S_Λ.

In the FRG formulation, on the other hand, the entire functional integral is performed "at once", but now explicitly equipped with a further infrared (IR) regularization in the form of a low-momentum cutoff depending a scale k that is introduced by replacing the bare action S_Λ in (33) by $S_{k,\Lambda} := S_\Lambda + \Delta S_k$, with $\Delta S_k[\chi] := \chi \cdot \mathcal{R}_k(-\nabla^2) \cdot \chi$. In terms of a spectral representation, the regulator kernel $\mathcal{R}_k(p^2) = k^2 r(\frac{p^2}{k^2})$ is required to satisfy the following general properties (see Appendix E of [89])

Reg (i) $\mathcal{R}_k(p^2) \to 0$ for $k \to 0$, ensuring that the $k \to 0$ limit of the various functionals coincide with their usual definitions.

Reg (ii) $\mathcal{R}_k(p^2) \sim k^2$ for $p^2 \lesssim k^2$, giving an effective $O(k^2)$ mass to the slow-modes.

Reg (iii) $\mathcal{R}_k(p^2)$ approaches zero sufficiently fast for $p^2 \gg k^2$, thereby leaving the fast-modes to be integrated out in the functional integral without a suppression factor.

The generic form of the regulator function $\mathcal{R}_k$ and its derivative $k\partial_k \mathcal{R}_k$, appearing in the flow equations (35), (36), is depicted in Figure 3. Moreover, the quadratic nature of ΔS_k leads to the appealing one-loop structure of the flow equations (35), (36).

The generating functional $W_{k,\Lambda}[J]$ and Legendre effective action $\Gamma_{k,\Lambda}[\phi]$ now carry both IR and UV cutoffs in their definitions,

$$\begin{aligned} e^{W_{k,\Lambda}[J]} &:= \int \mathcal{D}\chi_\Lambda e^{-S_\Lambda[\chi]-\Delta S_k[\chi]+J\cdot\chi}\,, \\ \Gamma_{k,\Lambda}[\phi] &:= J_{k,\Lambda}[\phi]\cdot\phi - W_{k,\Lambda}\big|_{J=J_{k,\Lambda}[\phi]} - \Delta S_k[\phi]\,, \quad \frac{\delta W_k}{\delta J}\Big|_{J=J_{k,\Lambda}[\phi]} \stackrel{!}{=} \phi\,, \end{aligned} \tag{34}$$

and the associated flow equations, respectively the Polchinski and Wetterich equations, are obtained by differentiating (34) with respect to k,

$$k\partial_k W_{k,\Lambda}[J] = -\tfrac{1}{2}\mathrm{Tr}\Big\{k\partial_k\mathcal{R}_k\Big[\tfrac{\delta W_{k,\Lambda}}{\delta J}\tfrac{\delta W_{k,\Lambda}}{\delta J} + \tfrac{\delta^2 W_{k,\Lambda}}{\delta J\delta J}\Big]\Big\}\,, \tag{35}$$

$$k\partial_k\Gamma_{k,\Lambda}[\phi] = \tfrac{1}{2}\mathrm{Tr}\Big\{k\partial_k\mathcal{R}_k\cdot G_{k,\Lambda}[\phi]\Big\}\,, \quad [\Gamma^{(2)}_{k,\Lambda}[\phi]+\mathcal{R}_k]\cdot G_{k,\Lambda}[\phi] \stackrel{!}{=} \mathbf{1}\,. \tag{36}$$

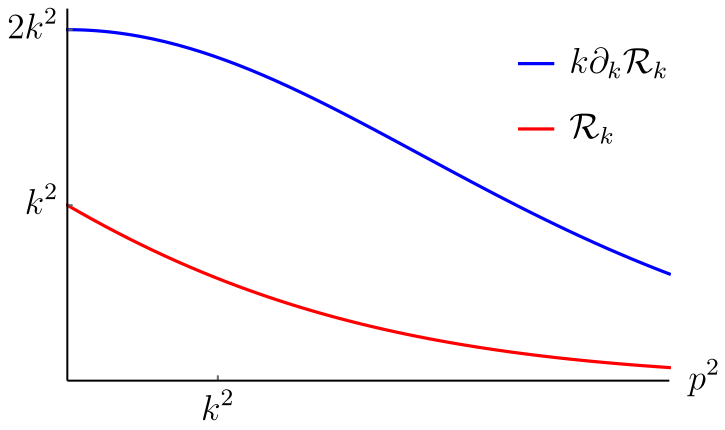


Figure 3: Shape of generic regulator function $\mathcal{R}_k$ and its derivative $k\partial_k\mathcal{R}_k$.

Importantly, both flow equations require specification of a boundary functional at some suitable k scale.

Modern applications focus on the flow of the Legendre effective action $\Gamma_{k,\Lambda}$, which has proven to be more robust in combination with truncation Ansätze. Further the boundary functional at $k = \Lambda$ can by-and-large be identified with a bare Wilsonian action S_Λ. Heuristically, this can be seen from the fact that for large $k = \Lambda$ the regulator adds a $O(\Lambda^2)$ mass term to the action, which leaves the integrand of the functional integral sharply peaked about the mean field ϕ. In a saddle-point evaluation, this yields S_Λ up to a doubly regularized trace-log term $\frac{1}{2}(\mathrm{Tr}\log)_{\Lambda,k}[S^{(2)} + \mathcal{R}_k]$. On the other hand, the regularized functional integral is meant to integrate momentum modes between the IR cutoff k and UV cutoff Λ. Thus, upon taking $k = \Lambda$, the doubly regularized trace-log term vanishes. In summary, $\Gamma_{k,\Lambda}$ interpolates between the bare action and the full effective action Γ_Λ according to

$$S_\Lambda \xleftarrow{k\to\Lambda} \Gamma_{k,\Lambda} \xrightarrow{k\to 0} \Gamma_\Lambda \,. \tag{37}$$

Importantly, (36) is purely kinematical in nature, with the dependence on the bare action S_Λ entering only through the initial condition $\Gamma_{\Lambda,\Lambda} = S_\Lambda$ (at large Λ). We note, however, that the flow of $\Gamma_{k,\Lambda}$ itself is typically not studied in the literature [63, 104, 82, 30, 74, 102, 89] as

therein the $\Lambda \to \infty$ limit is implicitly taken to yield the flow equation for $\Gamma_k := \lim_{\Lambda\to\infty} \Gamma_{k,\Lambda}$

$$k\partial_k \Gamma_k[\phi] \;=\; \tfrac{1}{2}\mathrm{Tr}\Big\{k\partial_k \mathcal{R}_k \cdot G_k[\phi]\Big\}\,, \quad [\Gamma_k^{(2)}[\phi] + \mathcal{R}_k]\cdot G_k[\phi] \stackrel{!}{=} \mathbf{1}\,, \tag{38}$$

with the claim that the RHS is well-defined without a UV regulator due to property **Reg (iii)** of the regulator kernel. This seemingly benign transition contains an important subtlety that is intimately tied to the issue of *UV renormalizablity*. Namely, **Reg (iii)** ensures that the transition from (36) to (38) follows rigorously if $\Gamma^{(2)}_{k,\Lambda}[\phi]$ is *independently* known to have a finite and non-trivial $\Lambda \to \infty$ limit. However, such a statement would require constructive control over the quantum field theory, which remains beyond reach in four dimensions. Accordingly, one has to be content with the following *if*...*then* statement (c.f. Appendix A.2 of [77])

> *If* there exists a sequence of initial actions $S_{n\Lambda_0}[\chi]$, $n \in \mathbb{N}$, such that the solution $\Gamma_{n\Lambda_0,k}[\chi]$ of (36) remains finite as $n \to \infty$, *then* the limit $\Gamma_k := \lim_{n\to\infty} \Gamma_{n\Lambda_0,k}$ obeys the UV-cutoff independent (38).

Conversely, given this premise, (38) should have at least one solution with a finite limit $\lim_{k\to\infty} \Gamma_k[\phi]$, which can be identified with the renormalized fixed point action since this object is the inverse limit of coarse graining. Note that in relation to (37), the limit $\Lambda \to \infty$ needs to be taken *at fixed* k, and only afterwards can k be made large.

As outlined in the Introduction, this standard FRG technique hinges strongly on Euclidean signature. On the other hand, for QFTs on an expanding Friedmann-Lemaître spacetime, Lorentzian signature seems indispensable. Although Lorentzian signature FRGs have been considered in Minkowski [94] and de Sitter [42] spacetimes, these constructions do not carry over to generic Friedmann-Lemaître spacetimes. The route taken here is to replace the covariant modulator by a merely spatial one through $\mathcal{R}_k(t,x;t',x') = \delta(t,t')R_k(t,x;t,x')$, while leaving the temporal dynamics unaffected. The Hessian $\Gamma_k^{(2)} + \mathcal{R}_k$ no longer possesses a local elliptic principal part, rendering the construction of an inverse $G_k[\phi]$ in (36) non-trivial and non-unique. The specialization to Friedmann-Lemaître spacetimes is detailed in Chapter 6. For spatially homogeneous mean-fields $\phi(t)$, the resulting flow equation reads

$$k\partial_k \Gamma_k[\phi] = -\frac{i\hbar}{2}\int dt d^d x\, N a^d \int \frac{d^d p}{(2\pi)^d} k\partial_k R_k(t,p) G_k[\phi](t,p)\,. \tag{39}$$

Here N and a refer to the Friedmann-Lemaître line-element $ds^2 = -N(t)^2dt^2 + a(t)^2\delta_{ij}dx^i dx^j$. Further, by slight abuse of notation, $G_k[\phi](t,p)$ in (39) is the temporal coincidence limit of the spatially Fourier transformed Green function in (36). For brevity we shall refer to (39) as the FLFRG. It still requires specification of a boundary functional in the UV. Guided by (37) we shall take the one-loop corrected bare action on the Friedmann-Lemaître background as the UV boundary functional. The counterterms are obtained from studying the associated one-loop effective action, which we show in Section 6.2 indeed has a finite $\Lambda \to \infty$ limit. This holds in a Wilsonian sense for a general (even) pure scalar potential $U(\phi)$, that however, necessitates the inclusion of an infinite tower of couplings to the Ricci scalar R. The one-loop renormalization of this system is analyzed in detail, with the notable feature that the spatial averaging induces an additional running of the Newton constant. With these boundary conditions specified, the flow (39) can be studied through suitable truncation Ansätze.

This requires some degree of analytic control over $G_k[\phi]$ as a functional of ϕ for not necessarily large k. Of course, the $G_k[\phi](t,p)$ cannot be computed in closed form even for a conceptually given Hessian. The spatial hopping expansion in Chapter 2 circumnavigates this problem. The other route is to use a simple truncation Ansatz (known as the Local Potential Ansatz, or LPA) wherein Γ_k is taken to be of the same form as the bare action, with k-dependent coupling functions whose flow is studied. The computation of $G_k[\phi]$ for large k can be based on the general aforementioned one-loop computation. The extension to small k is non-trivial for several reasons: It is here where the state dependence enters, and a suitable Hadamard state needs to be constructed in the first place, see Figure 2. Even once this is in place, analytical control over the ϕ dependence is technically challenging.

2.0 The Anti-Newtonian Expansion

2.1 Introduction

Inflationary cosmology maintains validity of the classical Friedmann-Lemaître (FL) equations of general relativity for all stages of the cosmological evolution following the brief quantum gravity epoch after the Big Bang, but sacrifices the strong energy condition. This allows one to successfully address several puzzles of standard FL cosmology, but introduces others in return: (i) based on the FL equations the inflationary period *must* be prefaced by a period of non-accelerated expansion immediately following the Big Bang, where kinetic rather than potential energy dominates. This can be seen in several complementary ways: the inflationary period is geodesically incomplete and postulating (necessarily fine-tuned) data at its beginning begs the question as to their origin. For single field inflation with only minor constraints on the potential the structure of the FL equations themselves enforces a stiff-fluid behavior near the Big Bang [38]. This fits within the broad class of inhomogeneous quiescent cosmologies [2, 49]. (ii) Quantum aspects are usually incorporated on the level of free fields on a classical FL background. The free fields arise from the quadratic part of the inflaton coupled Einstein-Hilbert action and factorize into the well-known scalar, vector, and tensor fluctuations. As far as the inflaton is concerned, a quadratic potential is disfavored by PLANCK data. For non-quadratic potentials the expansion around a FL background will produce a self-interacting scalar field theory with potential

$$U(\varphi+\chi) = U(\varphi) + U'(\varphi)\chi + \sum_{n\geq 2}\frac{1}{n!}U^{(n)}(\varphi)\chi^n\,. \tag{40}$$

The leading term is part of the FL background dynamics, the linear term cancels on account of the FL equations, all others remain. Beyond quadratic order in the fluctuations one is usually limited to perturbation theory. In addition to perturbation theory's intrinsic limitations it is also physically less suited in a cosmological context where the spatial inhomogeneities on different scales are of primary interest, while the nature of the (inflaton) potential is secondary and inferred. On a conceptual level, this together with the subdominance of spatial

gradients in the approach to the Big Bang in the BKL scenario [12, 13], suggests a spatial gradient expansion for QFTs on Friedmann-Lemaître backgrounds. Since continuum gradient expansions are technically problematic, a lattice version of a spatial gradient expansion (spatial hopping expansion) will be developed here. Compared to standard quantum field theoretical techniques it has the following advantages:

(i) The cosmological time can be kept continuous and real; this avoids notorious issues with Wick rotation (which is not well-defined on generic Friedmann-Lemaître backgrounds, see [6]) and temporal discretization.

(ii) In this spatially discretized setting, the scalar QFT under consideration reduces to two decoupled problems: (I) a combinatorial problem (the implementation of the spatial hopping expansion), and (II) a quantum mechanical problem (the self-interacting 'cosmological Quantum Mechanics'), which seeds the spatial hopping expansion.
Due to this decoupling, however, the specification of a potential (77) can be postponed, as can be the solution for the lowest order input data.

In this chapter we present the graph theoretical techniques for the solution of the above combinatorial problem in a cosmological setting. Indeed, much of technology carries over from the covariant Euclidean signature, presented in Chapter 3, with physically significant but technically easily traceable modifications. The solution of the explicitly time dependent 'cosmological Quantum Mechanics' is beyond the scope of this thesis. Importantly, however, arbitrary polynomial self-interactions may be included without immediately having to worry about (non-)renormalizeability. Moreover, backpropagated close to the Big Bang the quantum mechanical correlation functions are expected to simplify. At later times a variety of perturbative and non-perturbative techniques are available for quantum mechanical systems with time-dependent Hamiltonians, which should render (II) above more tractable than the full QFT.

2.2 Scalar field action and its hopping decomposition

Consider the action of a self-interacting scalar field theory on a spatially flat Friedmann-Lemaître background with line element $ds^2 = -N(t)^2dt^2 + a(t)^2\delta_{ij}dx^idx^j$ (in shift $N^a \equiv 0$ gauge),

$$\begin{aligned} S[\varphi] &= -\int d^D y\sqrt{-g}\Big\{\frac{1}{2}g^{\mu\nu}\partial_\mu\varphi\partial_\nu\varphi + \xi(\varphi)R(g) + U(\varphi)\Big\} \\ &= \int_{t_i}^{t_f} dt \int_\Sigma dx \Big\{\frac{1}{2n(t)}(\partial_t\varphi)^2 - n(t)a(t)^{2d}[U(\varphi) + \xi(\varphi)R(g^{\mathrm{FL}})] \\ &- \frac{1}{2}n(t)a(t)^{2d-2}\delta^{ij}\partial_i\varphi\partial_j\varphi\Big\}\,, \end{aligned} \tag{41}$$

where ξ and U are real analytic potentials, and $n = Na^{-d}$ is the lapse anti-density. In the second line, $R(g^{\mathrm{FL}})$ is the Ricci scalar of the Friedmann-Lemaître line element,

$$R(g^{\mathrm{FL}}) = 2d\frac{(N^{-1}\partial_t)^2 a}{a} + d(d-1)\frac{(N^{-1}\partial_t a)^2}{a^2}\,. \tag{42}$$

The form of the line element is preserved under $\mathrm{Diff}[t_i, t_f] \times \mathrm{ISO}(d)$ transformations, where the rotation group acts as global $\mathrm{Diff}(\Sigma)$ transformations connected to the identity. Under temporal reparameterizations $a(t)$ and $\varphi(t,x)$ transform as scalars, while $N(t)$ and $n(t)$ are temporal densities, $n'(t') = n(t)/|\partial t'/\partial t|$ etc. This is such that $\int_{t_i}^{t_f} dt\, N(t)a(t)^p = \int_{t_i}^{t_f} dt\, n(t)a(t)^{p+d}$ is invariant for any p. Finally, we remark that according to the standard "QFT on curved backgrounds" viewpoint, the geometry is treated as external, i.e. $n(t)$ and $a(t)$ are freely prescribed functions that are not required to satisfy any field equations. Alternatively, one may study "classically consistent cosmologies" wherein the spatially homogeneous part of φ is expected to act as a matter source that affects the geometry through the Einstein equations.

Suitably interpreted the second and third lines in the Friedmann-Lemaître action (41) carry different weights under a spatial scale transformation. To elucidate this, we view (41) as the matter part of a gravity-matter action, where the former comes with an overall inverse power of Newton's constant κ_G. This motivates the following redefinition

$$\bar\varphi \;=\; \sqrt{\kappa_G}\varphi\,, \quad U(\varphi) = \frac{1}{\kappa_G}\bar U(\bar\varphi)\,, \tag{43}$$

where $\bar{\varphi}$ is dimensionless and $\bar{U}(\bar{\varphi})$ has length dimension -2. When expressed in terms of $\bar{\varphi}, \bar{U}(\bar{\varphi})$ the matter action (41) carries an overall $1/\kappa_G$ pre-factor. In this form, consider the following scale transformation

$$\kappa_G \mapsto \lambda^d \kappa_G \,, \quad a(t) \mapsto \lambda a(t) \,, \quad \bar{\varphi} \mapsto \bar{\varphi} \,, \quad N \mapsto N \,, \tag{44}$$

for some $\lambda > 0$. It may be verified that this leaves the (reinterpretted) second line of (41) unchanged, while the third line gains an additional factor of λ^{-2}. On the otherhand, at the level of the line element $ds^2 = -N(t)^2 dt^2 + a(t)^2 \delta_{ij} dx^i dx^j$ the scale transformation enhances spacelike distances compared to timeline ones. This makes it harder to travel from one world-line to a neighboring world-line, equivalently the light cones appear to be squeezed for large λ. This is opposite to the familiar "post-Newtonian" scaling where the light cones are flattened to almost hypersurfaces of equal absolute time (i.e. the speed of light going to infinity). An expansion in powers of λ^{-2} can therefore be seen as an **Anti-Newtonian expansion**. Without referring to the scale transformation, the same rationale holds true for an expansion in powers of the spatial gradient term $-\frac{1}{2} n(t) a(t)^{2d-2} \delta^{ij} \partial_i \varphi \partial_j \varphi$ in (41).

As mentioned above, continuum gradient expansions are technically problematic, hence we proceed with a lattice version thereof. The implementation of a spatial hopping expansion proceeds as follows. In a first step we discretize the flat spatial sections Σ into a hypercubical lattice $(a_s \mathbb{Z})^d$ with spacing a_s. The discretization of the spatial gradient term is straightforward as the coefficient of $\delta^{ij} \partial_i \varphi \partial_j \varphi$ in (41) is only time dependent, so upon discretization,

$$\delta^{ij} \partial_i \varphi \partial_j \varphi \mapsto \frac{2d}{a_s^2} \varphi^2 - \frac{1}{a_s^2} \varphi (\ell^s \varphi), \tag{45}$$

where the spatial hopping matrix ℓ^s_{xy} acts by matrix multiplication on the discretized fields $\varphi(t, x)$ for fixed t. To make contact to the Functional Renormalization Group flow equations, we replace the nearest neighbor ℓ^s by a generic, potentially long ranged, hopping matrix

$$\ell_{xy} \in \mathbb{N}_0 \;\text{ for }\; \mathrm{dist}(x, y) > 0 \,, \quad \ell_{xx} = 0 \,. \tag{46}$$

For bookkeeping purposes we also multiply ℓ_{xy} by a pseudo-hopping parameter $\check{\kappa}$ ('pseudo', because the hopping parameter proper normally refers to a dimensionless reformulation of

Euclidean ϕ_4^4 theory). The discretized counterpart of (41) then reads

$$\begin{aligned} S[\varphi] &= \sum_{x\in\Sigma} a_s^d \int_{t_i}^{t_f} dt \left\{ \frac{1}{2n}(\partial_t\varphi)^2 - \frac{1}{2} n a^{2d-2} \frac{2d}{a_s^2}\varphi^2 - n a^{2d}[U(\varphi) + \xi(\varphi) R(g)] \right\}(t,x) \\ &+ \frac{1}{2}\check{\kappa} \int_{t_1}^{t_2} dt \sum_{x\in\Sigma} a_s^{d-2} n(t) a(t)^{2d-2} \varphi(t,x)(\ell\varphi)(t,x)\,. \end{aligned} \tag{47}$$

Structurally, this is of the form

$$S[\varphi] = \sum_{x\in\Sigma} s[a_s^{d/2}\varphi(\cdot,x)] + \check{\kappa}\mathcal{V}[\varphi], \tag{48}$$

for some 1+0 dimensional action $s[\vartheta]$ invoking fields a single spatial site only,

$$s[\vartheta] := \int_{t_1}^{t_2} dt \left\{ \frac{1}{2n}(\partial_t\vartheta)^2 - \frac{1}{2} n a^{2d-2} \frac{2d}{a_s^2}\vartheta^2 - n a^{2d}[U(\vartheta) + \xi(\vartheta) R(g)] \right\}, \tag{49}$$

and a hopping term $\mathcal{V}[\varphi]$ that connects different sites

$$\mathcal{V}[\varphi] := \frac{a_s^{d-2}}{2} \int_{t_i}^{t_f} dt\, n(t) a(t)^{2d-2} \sum_{x_1,x_2} \varphi(t,x_1)\ell_{x_1x_2}\varphi(t,x_2)\,. \tag{50}$$

The single site function $s[\vartheta]$, $\vartheta = \vartheta(t)$, can be viewed as the action of a quantum mechanical system. The decomposition (46) is the starting point for an Anti-Newtonian expansion: the expansion of a QFT around spatially decoupled (but in general self-interacting) quantum mechanical systems.

2.2.1 Generating functionals

We introduce two different generating functionals for the QFT with action (47) : the free energy $W[J]$ generating *connected* correlation functions, and the Legendre effective action $\Gamma[\phi]$ generating *one-particle irreducible* correlation functions. Each reduces for $\check{\kappa} = 0$ to sums of decoupled quantum mechanical generating functionals, denoted by $\omega[\jmath], \gamma[\varphi]$, respectively. Although the quantum mechanical quantities may be accessed through means other than a path integral, to introduce the relevant concepts it is nevertheless convenient to refer to an underlying path measure, formally written as $d\mu(\vartheta) = \mathcal{D}\vartheta \exp \frac{i}{\hbar} s[\vartheta]$. Copies of this quantum mechanical measure occur for each spatial lattice point and we write $\mu_x(\varphi) = d\mu(a_s^{d/2}\varphi(\cdot,x))$,

$x \in (a_s\mathbb{Z})^d$. In terms of this we represent the free energy functional as

$$e^{-\frac{i}{\hbar}W[J]} = \int \prod_{x\in\Sigma} \Big\{ d\mu_x(\varphi) e^{-\frac{i}{\hbar}a_s^d \int dt n(t) a(t)^{2d} \varphi(t,x) J(t,x)} \Big\} e^{\frac{i}{\hbar}\check{\kappa}\mathcal{V}[\varphi]}\,, \tag{51}$$

where the parameter $\check{\kappa}$ has been introduced to count powers of the hopping matrix ℓ. The induced $\check{\kappa}$ dependence is normally not indicated explicitly; occasionally we write $W_{\check{\kappa}}[J]$ for $W[J]$, and similarly for other functionals. Note that $J(t,x)$ must transform for each x as a temporal scalar.

Without a hopping term, *i.e.* for $\check{\kappa} = 0$, the functional integrals (51) factorize

$$W_0[J] = \sum_{x\in\Sigma} \omega\big[a_s^{d/2} J(\cdot,x)\big], \quad e^{-\frac{i}{\hbar}\omega[\jmath]} = \int d\mu(\vartheta) \exp\Big\{ -\frac{i}{\hbar} \int_{t_i}^{t_f} dt\, n(t) a(t)^{2d} \vartheta(t) \jmath(t) \Big\}. \tag{52}$$

By definition the moments of $\omega[\jmath]$ are the connected correlation functions of the associated quantum mechanical system,

$$\omega[\jmath] = \omega[0] + \sum_{n\geq 1} \frac{(i\hbar)^{(n-1)}}{n!} \int ds_1 \dots ds_n\, \mathrm{g}_n^c(s_1,\dots,s_n)\, \jmath(s_1)\dots\jmath(s_n)\,. \tag{53}$$

Normalizations for functional derivatives:

Since the flow equations and graph rules presented in the following section are expressed in terms of functional derivatives of W and Γ, we fix normalizations here. A covariant source coupling

$$\int dy\, \sqrt{g(y)} J(y)\phi(y) = \int dt dx N\sqrt{\mathrm{g}} J(t,x)\phi(t,x) = \int dt\, n(t) a(t)^{2d} \int dx\, J(t,x)\phi(t,x) \tag{54}$$

in the continuum suggests to define

$$\lim_{\epsilon\to 0} \frac{1}{\epsilon}(F[J+\epsilon H] - F[J]) = a_s^d \sum_x \int dt\, n(t) a(t)^{2d} H(t,x) \frac{\delta F[J]}{\delta J(t,x)} =: H \cdot \frac{\delta F}{\delta J}\,, \tag{55}$$

where the measure contribution is taken out of the functional derivative. Often a condensed notation is convenient, where the "$\cdot$" refers to a summation $a_s^d \sum_x$ and integration $\int dt n(t) a(t)^{2d}$ that emulates generalized matrix multiplications and traces. The definition (55) is such that for the source term in (51) it produces the unadorned $\varphi(t,x)$ as its functional derivative. Generally, $\delta F/\delta J(t,x)$ transforms as a temporal scalar and has length dimension $[\delta F/\delta J] = -(d+1) - [J] = -(d-1)/2$, for any dimensionless covariant functional $F[J]$. As

a mnemonic we note

$$\frac{\delta}{\delta J(t,x)} = \frac{1}{a_s^d n(t) a(t)^{2d}} \Big(\frac{\delta}{\delta J(t,x)} \Big)_{\text{naive}} , \tag{56}$$

and similarly (without the $1/a_s^d$) for $\delta/\delta\jmath(t)$. The naive derivatives obey the finite dimensional differentiation rules but are not covariantly defined. Defined as in (55) a $\vartheta(t)$ insertion into the second equation of (52) results from $i\hbar\delta/\delta\jmath(t)$, while a $\varphi(t,x)$ insertion into (51) is produced by $i\hbar\delta/\delta J(t,x)$. We introduce the shorthand notation

$$\begin{aligned} a_s^{\frac{md}{2}} \frac{\delta^m W_0[J]}{\delta J(t_m,x)\dots\delta J(t_1,x)} &= \frac{\delta^m \omega[\jmath]}{\delta\jmath(t_m)\dots\delta\jmath(t_1)}\Big|_{\jmath(\cdot)\mapsto a_s^{d/2} J(\cdot,x)} \\ &=: \omega_m(t_m,\dots,t_1|x)\,. \end{aligned} \tag{57}$$

The 'connected', source dependent quantum mechanical correlators ω_m are dimensionless and transform for fixed x as temporal scalars, $\omega'_m(t'_m,\dots,t'_1|x) = \omega_m(t_m,\dots,t_1|x)$, with $t' = t'(t)$. While temporal translation invariance is of course lost on a generic Friedmann-Lemaître background, one expects the ω_m to decay rapidly for large relative t_i's and to have at most integrable singularites when two coincide.

Next, we consider the Legendre effective action $\Gamma[\phi]$, i.e. the Legendre transform of $W[J]$. For our purposes a slightly modified definition is useful:

$$\Gamma[\phi] := \phi\cdot J[\phi] - W[J[\phi]] - \check\kappa\mathcal{V}[\phi]\,, \qquad \frac{\delta W}{\delta J}\big(J[\phi]\big) = \phi\,, \tag{58}$$

with a $\check\kappa$-independent mean field ϕ. The "$\cdot$" refers to the condensed notation in (55), i.e. a summation $a_s^d\sum_x$ and integration $\int dt n(t)a(t)^{2d}$ that emulates generalized matrix multiplications and traces. The leading, $\check\kappa$ independent term, then is the above Γ_0. Explicitly,

$$\Gamma_0[\phi] = \sum_x \gamma[a^{d/2}\phi(\cdot,x)]\,, \qquad \gamma[\varphi] = \varphi\cdot\jmath[\varphi] - \omega[\jmath[\varphi]], \qquad \frac{\delta\omega}{\delta\jmath}(\jmath[\varphi]) = \varphi\,. \tag{59}$$

The effective action $\Gamma[\phi]$ codes the complete information about the QFT under consideration but more efficiently than $W[J]$. Its functional derivatives generate the "vertex functions" linked to the moments of $W[J]$ by algebraic relations.

2.3 Hopping flow equations, recursion relations, and graph rules

Being quadratic in the fields the hopping interaction $\mathcal{V}[\varphi]$ in (50) can be viewed as a mode modulator akin to the ones externally introduced in the Functional Renormalization Group (FRG) approach. The pseudo hopping parameter $\check{\kappa}$ merely modulates the amplitude of the hopping term, but it can equally well serve as a control parameter. Differentiating (51) with respect to $\check{\kappa}$ one finds

$$\partial_{\check{\kappa}} W[J] = -\frac{a_s^{d-2}}{2} \sum_{x,x'} \ell_{xx'} \int_{t_i}^{t_f} dt\, n(t) a(t)^{2d-2} \Big\{ i\hbar \frac{\delta^2 W[J]}{\delta J(t,x)\delta J(t,x')} + \frac{\delta W[J]}{\delta J(t,x)} \frac{\delta W[J]}{\delta J(t,x')} \Big\} . \quad (60)$$

Here we used

$$\frac{\delta W[J]}{\delta J(t,x)} = \langle \varphi(t,x) \rangle_J \,, \quad \frac{\delta^2 W[J]}{\delta J(t,x)\delta J(t',x')} = \langle \varphi(t,x)\varphi(t',x') \rangle_J \,, \quad (61)$$

where $\langle\, \cdot\, \rangle_J$ denotes normalized functional averages with the source extended measure from (51). Anticipating that the temporal coincidence limits are unproblematic upon expansion, one sees that (60) is invariant under temporal reparameterizations, precisely because the correlators (61) are scalars. Inserting the power series ansatz

$$W[J] = W_0[J] + \sum_{l\geq 1} \frac{\check{\kappa}^l}{l!} W_l[J] \,, \quad (62)$$

converts (60) into the recursion

$$W_{l+1}[J] = -\frac{a_s^{d-2}}{2} \sum_{x,x'} \ell_{xx'} \int_{t_i}^{t_f} d\nu(t) \Big\{ i\hbar \frac{\delta^2 W_l}{\delta J(t,x)\delta J(t,x')} + \sum_{m=0}^{l} \binom{l}{m} \frac{\delta W_m}{\delta J(t,x)} \frac{\delta W_{l-m}}{\delta J(t,x')} \Big\} . \quad (63)$$

Throughout, the reparameterization invariant temporal measure $d\nu(t) = dt n(t) a(t)^{2d-2}$ will occur. Clearly, the combinatorics of the recursion is the same as in flat space; the structure of the terms generated as well as the numerical prefactors of the ω_n's. The only difference is that the non-trivial temporal measure $d\nu(t)$ replaces the translation invariant one dt. For the first three orders one has explicitly

$$W_1[J] \;=\; -a_s^{-2} \int_{t_i}^{t_f} d\nu(t) \sum_{x_1,x_2} \frac{1}{2} \ell_{x_1 x_2}\, \omega_1(t|x_1)\omega_1(t|x_2) \,,$$

$$
\begin{aligned}
W_2[J] &= a_s^{-4}\int_{t_i}^{t_f} d\nu(t)d\nu(s)\Big\{\frac{i\hbar}{2}\sum_{x_1,x_2}(\ell_{x_1x_2})^2\,\omega_2(t,s|x_1)\omega_2(s,t|x_2)\\
&+ \sum_{x_1,x_2,x_3}\ell_{x_1x_2}\ell_{x_2x_3}\,\omega_1(t|x_1)\omega_2(t,s|x_2)\omega_1(s|x_3)\Big\},\\
W_3[J] &= -a_s^{-6}\int_{t_i}^{t_f} d\nu(t)d\nu(s)d\nu(s')\Big\{\frac{(i\hbar)^2}{2}\sum_{x_1,x_2}(\ell_{x_1x_2})^3\,\omega_3(t,s,s'|x_1)\omega_3(t,s,s'|x_2)\\
&+ 3i\hbar\sum_{x_1,x_2,x_3}(\ell_{x_1x_2})^2\ell_{x_2x_3}\,\omega_2(t,s|x_1)\omega_3(t,s,s'|x_2)\omega_1(s'|x_3)\\
&+ i\hbar\sum_{x_1,x_2,x_3}\ell_{x_1x_2}\ell_{x_2x_3}\ell_{x_3x_1}\,\omega_2(t,s|x_1)\omega_2(s,s'|x_2)\omega_2(s',t|x_3)\\
&+ 3\sum_{x_1,x_2,x_3,x_4}\ell_{x_1x_2}\ell_{x_2x_3}\ell_{x_3x_4}\,\omega_1(s|x_1)\omega_2(s,t|x_2)\omega_2(t,s'|x_3)\omega_1(s'|x_4)\\
&+ \sum_{x_1,x_2,x_3,x_4}\ell_{x_1x_2}\ell_{x_1x_3}\ell_{x_1x_4}\,\omega_3(t,s,s'|x_1)\omega_1(t|x_2)\omega_1(s|x_3)\omega_1(s'|x_4)\Big\}. \qquad (64)
\end{aligned}
$$

At higher orders the recursive evaluation quickly becomes intractable. The recursion can however be solved in graph theoretical terms and results in a modification of the graph rules for the hopping expansion in flat Euclidean space [105]:

Graph rules for $W[J]$'s spatial hopping expansion:

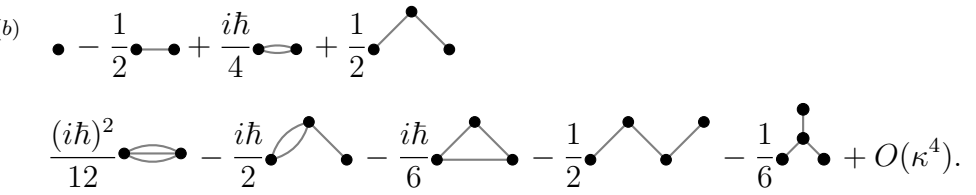
(a) At order $l \geq 1$ draw all topologically distinct connected graphs $C = (V, E) \in \mathcal{C}_l$ with $l = |E|$ edges connecting $2, \ldots, l+1$ vertices. Assign a dummy label i to each vertex and a dummy label e to each edge.

(b) Multiply by $l!(i\hbar)^{c(C)}/\mathrm{Sym}(C)$, where $\mathrm{Sym}(C)$ is the symmetry factor of the graph and $c(C)$ is its cyclomatic number (number of loops).

(c) To each graph a weight $\mu^W(C)$ is assigned as follows: a vertex i of degree n is attributed a weight $\omega_n(e_n, \ldots, e_1|i)$, evaluated on $a^{d/2}J(\cdot, i)$, where $e_n, \ldots, e_1$ are the labels of the incident edges. An edge connecting i, j is attributed a factor $-\ell_{ij}/a_s^2$.

(d) Embed the graph into $\Lambda^{|V|} \times \mathbb{R}^{|E|}$ by associating each vertex with a unique spatial lattice point, $i \mapsto x_i \in \Lambda$, $i = 1, \ldots, |V|$, the same lattice point may occur several times. Associate to each edge label a unique real time variable, $e \mapsto t_e \in \mathbb{R}$, $e = 1, \ldots, l = |E|$. Perform an unconstrained sum over all $x_1, x_2, \ldots, x_{|V|}$ and an unconstrained integration over all $t_1, \ldots, t_l$, with temporal measures $d\nu(t_1), \ldots, d\nu(t_l)$.

For illustration consider the graphs in (a) divided by their symmetry factors in (b) to $O(\kappa^3)$:

$W[J] \overset{(a),(b)}{=}$  (65)

Upon application of steps (c), (d) this matches the recursively computed result in (64). Generally, the result of (a), (b), (c) of the graph rule can be recast symbolically as:

$$\sum_{C=(V,E)\in\mathcal{C}_l} \frac{(-)^l l!(i\hbar)^{c(C)}}{\mathrm{Sym}(C)} \prod_{e\in E} \ell_{\theta(e)} \prod_{v\in V} \omega_{d(v)}(e_{d(v)},\dots,e_1|v)\,, \tag{66}$$

where the double product comprises $(-)^l\mu^W(C)$. The graph sum is over all connected graphs $C=(V,E)$ with $|E|=l$ edges, $\theta(e)$ is the unordered pair of vertices connected by e, and $d(v)$ is the number of incident lines at vertex v. The definitions of the symmetry factor $\mathrm{Sym}(C)$ and the cyclomatic number $c(C)$ of C are standard, see the graph theory glossary in Section 3.2.1. Using for simplicity the same symbol $\mu^W(C)$ to denote the weight after embedding into $\Lambda^{|V|}\times\mathbb{R}^{|E|}$, the averaging from (d) gives the final result:

$$W_l[J] = a_s^{-2l} \sum_{C=(V,E)\in\mathcal{C}_l} \frac{(-)^l l!(i\hbar)^{c(C)}}{\mathrm{Sym}(C)} \sum_{x_1,\dots,x_{|V|}} \int d\nu(t_l)\dots d\nu(t_1)\,\mu^W[C]\,. \tag{67}$$

This concludes our presentation of the graph rules for the free energy $W[J]$.

The transition to the effective action Γ_κ proceeds via (58), and the Wetterich equation for Γ_κ can be obtained along the usual lines, replacing the Polchinski type (60). As in (60) we take $\check\kappa$ as the control parameter and regard the Wetterich equation as describing the flow in $\check\kappa$. For Euclidean signature on a hypercubic lattice no complications arise in the transition. Since $\mathcal{V}$ in (48) contains fields at the same time, one will initially replace it with a temporally point split version $\check{\mathcal{V}}$ with kernel $\check\ell(t,x;t',x')$. The resulting "hopping FRG" reads

$$\partial_{\check\kappa}\Gamma[\phi] = \frac{i\hbar}{2} a_s^{d-2} \sum_{x,y\in(a_s\mathbb{Z})^d} \int d\nu(t)\,d\nu(s)\check\ell(t,x;s,y)[\Gamma^{(2)}(\phi)+\check\kappa\check\ell\,]^{-1}(t,x;s,y)\,, \tag{68}$$

where we recall that $d\nu(t) = dt\,n(t)a(t)^{2d-2}$ is the reparameterization invariant temporal measure. The temporal coincidence limit as the original hopping term is restored,

$\check{\ell}(t,x;s,y) \mapsto \ell_{xx}\delta(t-t')n(t)^{-1}a(t)^{-2d+2}$, can be shown to exist termwise in the $\check{\kappa}$-expansion of (68). The key aspect is that $\ell_{xx'} = 0$ for $x = x'$, which precludes the occurrence of products of temporal delta functions. This limit also restores the exact – not mode-modulated – quantum mechanical dynamics. With this interpretation of (68) in place, the main deviation from the standard uses is that the initial conditions are imposed at the ultralocal, $\check{\kappa} = 0$, scale

$$\Gamma[\phi]\big|_{\check{\kappa}=0} \stackrel{!}{=} \Gamma_0[\phi] = \sum_{x\in(a_s\mathbb{Z})^d} \gamma[a_s^{d/2}\phi(\,\cdot\,,x)]\,. \tag{69}$$

For the expansion we use the normalizations

$$\Gamma[\phi] = \Gamma_0[\phi] + \sum_{l\geq 1} \frac{\check{\kappa}^l}{l!}\Gamma_l[\phi]\,, \tag{70}$$

in parallel to (62). The leading $\check{\kappa}$ independent term is (69).

The expansion of the Wetterich equation (68) gives rise to a closed recursion for the Γ_l's. To low orders one finds

$$\begin{aligned}
\Gamma_2[\phi] &= a_s^{-4}\int d\nu(t_1)d\nu(t_2)\,\frac{i\hbar}{2}\sum_{x_1,x_2}(\ell_{x_1x_2})^2\,\varpi_2(t_1,t_2|x_1)\varpi_2(t_2,t_1|x_2)\\
\Gamma_3[\phi] &= -a_s^{-6}\int d\nu(t_1)d\nu(t_2)d\nu(t_3)\Big\{\frac{(i\hbar)^2}{2}\sum_{x_1,x_2}(\ell_{x_1x_2})^3\,\varpi_3(t_1,t_2,t_3|x_1)\varpi_3(t_1,t_2,t_3|x_2)\\
&+ i\hbar\sum_{x_1,x_2,x_3}\ell_{x_1x_2}\ell_{x_2x_3}\ell_{x_3x_1}\,\varpi_2(t_1,t_2|x_1)\varpi_2(t_2,t_3|x_2)\varpi_2(t_3,t_1|x_3)\Big\}
\end{aligned} \tag{71}$$

$$\begin{aligned}
\Gamma_4[\phi] &= a_s^{-8}\int d\nu(t_1)d\nu(t_2)d\nu(t_3)d\nu(t_4)\Big\{\frac{(i\hbar)^3}{2}\sum_{x_1,x_2}(\ell_{x_1x_2})^4\varpi_4(t_1,t_2,t_3,t_4|x_1)\\
&\times\ \varpi_4(t_1,t_2,t_3,t_4|x_2)\\
&+\ 6(i\hbar)^2\sum_{x_1,x_2,x_3}(\ell_{x_1x_2})^2\,\ell_{x_1x_3}\,\ell_{x_2x_3}\,\varpi_3(t_1,t_2,t_3|x_1)\,\varpi_3(t_1,t_2,t_4|x_2)\,\varpi_2(t_3,t_4|x_3)\\
&+\ 3(i\hbar)^2\sum_{x_1,x_2,x_3}(\ell_{x_1x_2})^2\,(\ell_{x_2x_3})^2\varpi_2(t_1,t_2|x_1)\varpi_2(t_3,t_4|x_3)\,\big[\varpi_4(t_1,t_2,t_3,t_4|x_2)\\
&-\ \int a(s_1)^2d\nu(s_1)a(s_2)^2d\nu(s_2)\varpi_3(t_1,t_2,s_1|x_2)\gamma_2(s_1,s_2|x_2)\varpi_3(s_2,t_3,t_4|x_2)\big]
\end{aligned}$$

$$+ \; 3i\hbar \sum_{x_1,x_2,x_3,x_4} \ell_{x_1x_2}\,\ell_{x_2x_3}\,\ell_{x_3x_4}\,\ell_{x_4x_1}\varpi_2(t_1,t_2|x_1)\varpi_2(t_2,t_3|x_2))$$
$$\times \; \varpi_2(t_3,t_4|x_3))\varpi_2(t_4,t_1|x_4)\Big\}\,. \tag{72}$$

Here the quantum mechanical correlators (57) now have the source dependence replaced by one on the mean field φ. We define

$$\omega_n(t_n,\ldots,t_1|x)\big|_{\jmath(\cdot)\mapsto a^{d/2}\frac{\partial\gamma}{\partial\varphi}(a^{d/2}\phi(\cdot,x))} =: \varpi_n(t_n,\ldots,t_1|x)\,,$$
$$\gamma_n(t_n,\ldots,t_1|x) := \frac{\delta^n\gamma}{\delta\varphi(t_n)\ldots\delta\varphi(t_1)}\,, \quad n\geq 2\,. \tag{73}$$

Again, these transform as scalars under temporal reparameterizations for fixed x. For $n=1$ we identify $\varpi_1(t|x)$ with $a_s^{d/2}\phi(t,x)$ and $\gamma_1(t|x)$ with $\jmath[\varphi](t,x)$.

However, beyond these low orders, the direct recursion quickly becomes intractable. To understand the structural aspects of the expansion, the following mixed recursion turns out to be advantageous (see (90) in Chapter 3 for the covariant version)

$$\Gamma_l[\phi] = -W_l[\Gamma_0^{(1)}]\Big|_{1\mathrm{PI}} - \sum_{m=2}^{l-2}\sum_{k=1}^{[m/2]} \sum_{\substack{m_1+\ldots+m_k=m\\ m_i\geq 1}} \frac{(l-m)}{lk!} W_{l-m}^{(k)}[\Gamma_0^{(1)}]\Big|_{1\mathrm{PI}} \cdot \Gamma_{m_1}^{(1)}\ldots\Gamma_{m_k}^{(1)}\,, \tag{74}$$

where the "$\cdot$" initially refers to $a_s^d\sum_{x_i}\int dt_i n(t_i)a(t_i)^{2d}$, $1\leq i\leq m$; these arise from a functional Taylor expansion of W. The recursion relation (74) then in principle determines all $\Gamma_l[\phi]$ with the original hopping interaction. This mixed recursion (74) can be solved in graph theoretical terms and then allows one to compute each Γ_l directly. The basic graph rules are an adaptation of the results in Chapter 3:

Graph rules for $\Gamma_l[\phi]$'s spatial hopping expansion:

(a) At order $l\geq 2$ draw all topologically distinct 1LI graphs with l edges, $L=(V,E)\in\mathcal{L}_l$. Assign a dummy label i to each vertex and dummy label e to each edge.

(b) Multiply by $l!(i\hbar)^{c(L)}/\mathrm{Sym}(L)$, where $\mathrm{Sym}(L)$ is the symmetry factor of the graph and $c(L)$ is its cyclomatic number (number of loops).

(c) To each graph a weight $\mu^\Gamma(L)$ is assigned as follows: an edge connecting vertices i,j is

attributed a factor $-\ell_{ij}/a_s^2$. A vertex i of degree n is attributed a factor $\mu_v^\Gamma(e_n,\dots,e_1|i)$, where $e_1,\dots,e_n$ are the edges incident on i.

(d) Embed the graph into $\Lambda^{|V|}\times\mathbb{R}^{|E|}$ by associating each vertex with a unique spatial lattice point, $i\mapsto x_i\in\Lambda$, $i=1,\dots,|V|$, the same lattice point may occur several times. Associate to each edge label a unique real time variable, $e\mapsto t\in\mathbb{R}$, $e=1,\dots,l=|E|$. Perform an unconstrained sum over all $x_1,x_2,\dots,x_{|V|}$ and an unconstrained integration over all $t_1,\dots,t_l$, with temporal measures $d\nu(t_1),\dots,d\nu(t_l)$.

The vertex functions μ_v^Γ are obtained from labelled tree graphs as described in Section 3.3. As in the present case the expansion is about a *spatially* ultralocal functional, the following modification is necessary: the ends of the dashed lines ending on open circles are given labels s_j. A dashed line with end labels s_1,s_2 connecting two open circles is attributed $\gamma_2(s_1,s_2|i)$, while a $m\geq 3$ valent dashed vertex is attributed a factor $\gamma_m(s_m,\dots,s_1|i)$. The labeled open circles are attributed factors of the form $\varpi_{n+m}(t_n,\dots,t_1,s_m,\dots,s_1|i)$, where the $t_1,\dots,t_n$ are associated with the full edges, and the $s_1,\dots,s_m$ are associated with the dashed edges. An unconstrained integral is to be performed over the time arguments associated with the dashed edges with temporal measure $a(t)^2d\nu(t)$.

As to the origin of the different temporal measures $d\nu(t)$ and $a(t)^2d\nu(t)$ associated with the full and dashed graphs (respectively) we recall that the dashed graphs are a systematic solution of the recursion system (74), as detailed in Chapter 3. The "$\cdot$" in (74) arises from a functional Taylor expansion, and hence comes with temporal measure $a(t)^2d\nu(t)$ due to the definition of the functional derivative in (55). The action of $\delta/\delta\varphi(s_{m+1})$ on $\gamma_m(s_m,\dots,s_1)$ produces $\gamma_{m+1}(s_{m+1},\dots,s_1)$, while its action on $\varpi_{n+m}(t_n,\dots,t_1,s_m,\dots,s_1)$ yields $\int a(s)^2d\nu(s)\varpi_{n+m+1}(s,\dots)\gamma_2(s,s_{m+1})$. This shows that each time label associated with the dashed graphs must be integrated with temporal measure $a(t)^2d\nu(t)$, not $d\nu(t)$.

For illustration, we present two examples of such vertex weights computed from the tree graph rule.

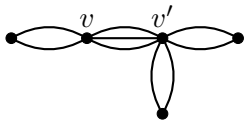
(i) The vertex v in the pair of glasses graph:

The weight of the labeled vertex v is

$$\varpi_4(t_1,t_2,t_3,t_4|v) - \int a(s_1)^2 d\nu(s_1) a(s_2)^2 d\nu(s_2) \varpi_3(t_1,t_2,s_1|v)\gamma_2(s_1,s_2|v)\omega_3(s_2,t_3,t_4|v)\,, \tag{75}$$

where t_1, t_2, t_3, t_4 are the time variables associated to the solid edges. Note that this coincides with the recursively computed weight in (72).

(ii) A more complicated graph with two articulation vertices is:



The weights of the labeled vertices v, v' are

$$\begin{aligned}
&\mu_v^\Gamma(t_1,t_2,t_3,t_4,t_5|v) = \varpi_5(t_1,t_2,t_3,t_4,t_5|v) \\
&- \int a(s_1)^2 d\nu(s_1) a(s_2)^2 d\nu(s_2) \varpi_3(t_1,t_2,s_1|v)\gamma_2(s_1,s_2|v)\omega_3(s_2,t_3,t_4,t_5|v)\,, \\
&\mu_{v'}^\Gamma(t_3,t_4,t_5,t_6,t_7,t_8,t_9|v') = \varpi_7(t_3,t_4,t_5,t_6,t_7,t_8,t_9|v') \\
&-2\int a(s_1)^2 d\nu(s_1) a(s_2)^2 d\nu(s_2) \varpi_3(t_6,t_7,s_1|v')\gamma_2(s_1,s_2|v')\omega_6(s_2,t_3,t_4,t_5,t_8,t_9|v') \\
&- \int a(s_1)^2 d\nu(s_1) a(s_2)^2 d\nu(s_2) \varpi_4(t_3,t_4,t_5,s_1|v')\gamma_2(s_1,s_2|v')\omega_5(s_2,t_6,t_7,t_8,t_9|v') \\
&+ \int a(s_1)^2 d\nu(s_1) a(s_2)^2 d\nu(s_2) a(s_3)^2 d\nu(s_3) a(s_4)^2 d\nu(s_4) \gamma_2(s_1,s_2|v')\gamma_2(s_3,s_4|v') \\
&\times \varpi_3(s_1,t_6,t_7|v')\varpi_3(s_4,t_8,t_9|v')\varpi_5(s_2,s_3,t_3,t_4,t_5|v') \\
&+2\int a(s_1)^2 d\nu(s_1) a(s_2)^2 d\nu(s_2) a(s_3)^2 d\nu(s_3) a(s_4)^2 d\nu(s_4) \gamma_2(s_1,s_2|v')\gamma_2(s_3,s_4|v') \\
&\times \varpi_3(s_4,t_8,t_9|v')\varpi_4(s_2,s_3,t_6,t_7|v')\varpi_4(s_1,t_3,t_4,t_5|v') \\
&+ \int a(s_1)^2 d\nu(s_1) a(s_2)^2 d\nu(s_2) a(s_3)^2 d\nu(s_3) \gamma_3(s_1,s_2,s_3|v')\varpi_3(s_1,t_6,t_7|v')\varpi_3(s_2,t_8,t_9|v') \\
&\times \varpi_4(s_3,t_3,t_4,t_5|v').
\end{aligned} \tag{76}$$

Here $t_1,\ldots,t_9$ and $s_1,\ldots,s_4$ are the time variables associated with the solid and dashed edges, respectively. Finally, from the definition of the functional derivative (55), it follows that the vertex functions μ_v^Γ are scalars under temporal reparametrizations.

2.4 Conclusions

We have presented the Anti-Newtonian expansion in a spatially discretized setting, where the flat spatial sections of the Friedmann-Lemaître background are replaced with a hypercubical lattice $(a_s\mathbb{Z})^d$ of spacing a_s. This discretized expansion amounts to a spatial hopping (linked cluster) expansion, expanding around spatially decoupled quantum mechanical systems, one associated with each lattice site. The rationale for the name "Anti-Newtonian" follows because this expansion around spatially decoupled systems may be conceptually associated with a scale transformation that at the level of the line element $ds^2 = -N(t)^2dt^2 + a(t)^2\delta ijdx^idx^j$ enhances spacelike distances compared to timelike ones. This makes it harder to travel from one world-line to a neighboring world-line, equivalently the light cones appear to be squeezed. This is opposite to the "post-Newtonian" scaling where the light cones are flattened to almost hypersurfaces of equal absolute time, and is hence referred to as Anti-Newtonian. In this framework, the solution of the QFT decouples into two sub-problems: (1) the solution of the cosmological quantum mechanics, conceptually associated with the decoupled wordlines in the Anti-Newtonian limit; and (2) the solution of the combinatorial problem that allows one to analytically control the terms of the linked cluster expansion, which is conceptually associated with restoring the spatial interaction between the neighboring world lines.

We have presented graph theoretical techniques for the solution of the combinatorial problem (2) associated to the spatial hopping expansions of the QFT generating functionals $W[J]$ and $\Gamma[\phi]$ on generic Friedmann-Lemaître spacetimes. We close this section by highlighting a number of key structural properties of the graph expansions:

(i) The graph rules for the spatial hopping expansion of $W[J]$ and $\Gamma[\phi]$ are to a large extent model independent. The form of the scalar potential $U(\varphi)$ does not enter, and the embedding of the abstract graphs into (the spatially discretized) spacetime occurs only in part (d) of both sets of graph rules.

(ii) The traditional hopping or linked cluster expansion mostly use connected graphs. The expansion of $\Gamma[\phi]$ in terms of one-line-irreducible (1LI) graphs leads to a considerable computational gain as there are far fewer 1LI graphs. For example, for edge-count

$l = 6$ there are 101 connected but only 22 1LI graphs.

(iii) A notable feature of the $\Gamma[\phi]$ as compared to those for $W[J]$ is the additional structure at the vertices encoded by the vertex weights μ_v^Γ. These are determined by purely *local* data, depending *only* on the structure of the abstract graph *at* the vertex v, through the pattern of incident subgraphs. As the same patterns reoccur in many 1LI graphs, the μ_v^Γ's need to be generated only once and can be stored in a look-up table.

(iv) After embedding the graphs into spacetime, the result characterizes the Legendre effective action Γ's nonlocality precisely to all orders.

3.0 Graph Rules for the Linked Cluster Expansion of the Legendre Effective Action

3.1 Introduction

The Legendre effective action is a central quantity in all areas of many-body quantum physics. In particular, it features prominently in the functional renormalization group approach based on the flow equation

$$\partial_k \Gamma_k = \frac{1}{2}\mathrm{Tr}\big\{\partial_k R_k [\Gamma_k^{(2)} + R_k]^{-1}\big\}\,, \tag{77}$$

describing its response to a modulation of the system's mode content set by the kernel R_k. The flow equation (77) is now being used in fields as diverse as: solid state physics, statistical physics, and quantum gravity, see [63, 104, 82] for book-sized accounts. The response (77) is itself kinematical in nature, dynamical information in injected exclusively through initial conditions. As a consequence, the results obtained are only as non-perturbative as the initial conditions are. An especially interesting choice of initial conditions are ultralocal ones as they can in a lattice formulation be be computed exactly from single site integrals [70]. A solution of (77) with such initial data, if feasible, will emulate a linked cluster or hopping expansion but with a scale dependent long-ranged interaction

$$S[\chi] = \sum_x s[\chi_x] + \frac{\kappa}{2}\sum_{x,y} \chi_y \ell_{xy}(k) \chi_x\,. \tag{78}$$

For definiteness we consider a self-interacting scalar field theory on a D-dimensional hypercubic lattice (identified with $\mathbb{Z}^D$) in a dimensionless formulation. Here, $s : \mathbb{R} \to \mathbb{R}$ is a function bounded from below that collects all terms from the original lattice action referring to a single site. The hopping parameter $\kappa > 0$ arises as a dimensionless combination of the original mass and coupling parameters and the lattice spacing. A fundamental lattice action would only connect nearest neighbors on the lattice through ℓ_{xy}. In order to obtain a solution of (77) we allow ℓ_{xy} to be long-ranged and be modulated by the control parameter

k. The details of the modulation are inessential in the following as we take κ as the control parameter and replace (77) by

$$\partial_\kappa \Gamma_\kappa = \frac{1}{2} \sum_{x,y} \ell_{xy} \big[\Gamma_\kappa^{(2)} + \kappa \ell\big]^{-1}_{xy} , \quad \Gamma_\kappa = \Gamma_0 + \sum_{l \geq 2} \kappa^l \Gamma_l[\phi] . \tag{79}$$

Here $\Gamma_0[\phi] = \sum_x \gamma(\phi_x)$, where γ and its derivatives γ_n are computable at a single site from s only. The $O(\kappa)$ term vanishes, $\Gamma_2[\phi] = -\frac{1}{4} \sum_{x,y} (\ell_{xy})^2 \gamma_2(\phi_x)^{-1} \gamma_2(\phi_y)^{-1}$, and all Γ_l, $l \geq 3$, are then determined recursively; see (511) in Appendix A. Importantly the series can be expected to have finite radius of convergence $\kappa < \kappa_c$; see the discussion below. Once the series (79) has been constructed, an in principle exact solution of (77) arises simply by substitution, $\Gamma_k = \Gamma_\kappa|_{\ell \mapsto \ell(k)}$.

The direct iteration (511) becomes, however, impractical beyond $O(\kappa^6)$ or so (both in manual computations and in automated symbolic implementations). The repeated functional differentiations of $\Gamma_0[\phi]$ lead to site identifications whose combinatorics is best recast in graph theoretical terms. The graph theoretical analysis of hopping expansions of course has a long history, see [105, 79, 52] and the references therein. The convergence proofs of generalized Mayer expansions typically rely on tree graph bounds [18]. In the computational uses of linked cluster expansions, the focus is normally on nearest neighbor interactions and quantities of direct interest for critical behavior like generalized susceptibilities [79, 52]; a convergence proof for them in scalar quantum field theory can be reduced to tree graph bounds [85]. The effective action Γ_κ can alternatively be defined as a (slightly modified) Legendre transform of the free energy functional W_κ. Graph theoretical rules for the linked cluster expansion of W_κ have originally been presented by Wortis [105] and will be briefly reviewed in Section 2. Graph theoretical expansions for $\Gamma_\kappa[\phi]$ have been discussed previously but do not cover the material presented here: the rules and results of [97, 98] hinge on specific features of the Ising model which do not generalize. Hybrid perturbative expansions have been considered in [26]. A relevant combinatorial Legendre transform has been studied in [53, 34] in a setting that emulates perturbation theory. Some of the results of [53] will reoccur in our analysis of Γ_0 in Appendix A. There are also abstract variants of a Legendre transform formulated in terms of combinatorial species [19, 34]. None of these seem to bear an obvious relation to our result.

We present the solution of the recursion implied by (79) in graph theoretical terms. Let $\mathcal{L}_l$ be the set of one-line irreducible connected graphs with l edges. For any $L = (V, E) \in \mathcal{L}_l$ and any vertex $v \in V$ consider the decomposition of L into one-vertex irreducible subgraphs, $|I(v)|$ of which each contain a copy of v. The set $B(v)$ of copies is used to label a class of *tree* graphs $\mathcal{T}(B(v), n), n = 1, \ldots, |I(v)|$. To each $T \in \mathcal{T}(B(v), n)$ two integers $s(T)$ and $\mathrm{Perm}B(v)/\mathrm{Sym}(T)$ are assigned, as detailed in Section 3.3. Then:

Theorem. For any $l \geq 2$ the exact solution of the recursion implied by (79), i.e. (511), is given by

$$\begin{aligned} \Gamma_l[\phi] &= \sum_{L=(V,E)\in\mathcal{L}_l} \frac{(-)^{l+1}}{\mathrm{Sym}(L)} \prod_{e\in E} \ell_{\theta(e)} \prod_{v\in V} \mu^\Gamma(v|B) \\ \mu^\Gamma(v|B) &= \sum_{n=1}^{|I(v)|} \sum_{T\in\mathcal{T}(B(v),n)} (-)^{s(T)} \frac{|\mathrm{Perm}(B(v))|}{\mathrm{Sym}(T)} \mu(T)\,. \end{aligned} \tag{80}$$

In the first line an unconstrained sum over the lattice points associated with the vertices is tacit. Further E is the edge list with $\theta(e)$ the pair of vertices connected by e, and $\mathrm{Sym}(L)$ is the symmetry factor of L. In the second line, $\mu(T)$ is a weight depending only on the value of ϕ at v.

This chapter is organized as follows. In Section 3.2.1 we summarize known graph rules for the free energy functional and set the terminology. A mixed recursion relation (98), equivalent to the one implied by (79) is derived in Section 3.2.2, and used to derive the first line of (80). The relevant class of labeled tree graphs is introduced in Section 3.3.1, the graph rules for $\mu^\Gamma(v|L)$ are formulated and illustrated in Section 3.3.2, and an all-order proof for their validity is given in Section 3.3.3. A simplified version of $\mu^\Gamma(v|B)$ obtained by performing subsums with fixed $\mu(T)$ is derived in Section 3.4. Appendix A presents explicit and independently computed results for $\Gamma_2, \ldots, \Gamma_5$, and discusses the single site data together with their combinatorics.

This chapter is based on [9].

3.2 From connected graphs to articulation vertices

For convenience we refer to expansions in powers of $\kappa\ell_{xy}$ (with $\ell_{xx} = 0$ but $\ell_{xy} \neq 0$ for $\mathrm{dist}(x, y) \geq 1$) as a long range hopping (LRH) expansion. The graph expansions considered have two main ingredients: first, a class of graphs with some partial order consistent with the order in κ. Second, a weight function that assigns to each graph of the class a numerical value depending on certain input data. In addition to ℓ_{xy} itself, the input data are always the derivatives $\omega_m(h) = \partial^m\omega/\partial h^m$ and/or $\gamma_m(\varphi) = \partial^m\gamma/\partial\varphi^m$ of the single site functions described in Appendix B. The class of graphs and the weight functions will depend on the quantity considered. The goal of this section is to reduce the problem of identifying the graph rules for Γ_κ's LRH expansion to the determination of the weight associated to articulation vertices.

3.2.1 Basics

The Γ_k flow equation (77) can be obtained as the Legendre transform of a Polchinski-type flow equation for W_k, the mode modulated free energy functional. For an action of the form (78) one may again take κ as the control parameter to obtain along the familiar lines

$$\partial_\kappa W_\kappa[H] = -\frac{1}{2}\sum_{x,y}\ell_{xy}\left\{\frac{\delta^2 W_\kappa[H]}{\delta H_x \delta H_y} + \frac{\delta W_\kappa[H]}{\delta H_x}\frac{\delta W_\kappa[H]}{\delta H_y}\right\}. \tag{81}$$

Here we impose ultralocal initial data $W_0[H] = \sum_x \omega(H_x)$, where $\omega(h)$ is determined by the single site action s in (78). The ansatz $W_\kappa[H] = W_0[H] + \sum_{l\geq 1}\kappa^l W_l[H]$ converts (81) into the recursive system

$$W_{l+1}[H] = -\frac{1}{2(l+1)}\sum_{x,y}\ell_{xy}\left\{\frac{\delta^2 W_l[H]}{\delta H_x \delta H_y} + \sum_{k=0}^{l}\frac{\delta W_k[H]}{\delta H_x}\frac{\delta W_{l-k}[H]}{\delta H_y}\right\}, \quad l \geq 0\,. \tag{82}$$

Explicitly, the first two orders read

$$\begin{aligned} W_1[H] &= -\frac{1}{2}\sum_{x,y}\ell_{xy}\frac{\delta W_0[H]}{\delta H_x}\frac{\delta W_0[H]}{\delta H_y}\,, \\ W_2[H] &= \frac{1}{2}\sum_{x,y,z,w}\ell_{xy}\ell_{zw}\,\frac{\delta^2 W_0[H]}{\delta H_y \delta H_w}\left\{\frac{1}{2}\,\frac{\delta^2 W_0[H]}{\delta H_x \delta H_z} + \frac{\delta W_0[H]}{\delta H_x}\frac{\delta W_0[H]}{\delta H_z}\right\}. \end{aligned} \tag{83}$$

The repeated $H_x, H_y, \ldots$, functional derivatives of $W_0[H]$ produce point identifications and coefficients that are source-dependent derivatives of the single-site generating function $\omega(h)$. The combinatorics of these point identifications is best formulated in graph theoretical terms. Such rules have been formulated and proven by Wortis [105]; the relation to a Polchinski-type flow equation was noted in [18] where subject to additional conditions also a convergence proof is given.

Graph rules for W[H]:

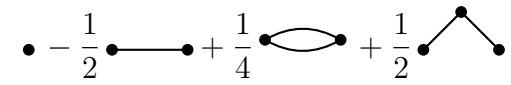
(a) At order $l \geq 1$ in κ draw all topologically distinct connected graphs $C = (V, E) \in \mathcal{C}_l$ with $l = |E|$ edges connecting $2, \ldots, l+1$ vertices. Assign a dummy label to each vertex.

(b) Divide by the symmetry factor $\mathrm{Sym}(C)$ of the graph.

(c) To each graph a weight $\mu^W(C)$ is assigned as follows: a vertex i of degree n is attributed a weight $\omega_n(H_i)$, an edge connecting i, j is attributed a factor $-\ell_{ij}$.

(d) Embed the graph into the lattice $\mathbb{Z}^D$ by associating each vertex with a unique lattice point, $i \mapsto x_i$, $i = 1, \ldots, |V|$, the same lattice point may occur several times. Perform an unconstrained sum over all $x_1, x_2, \ldots, x_{|V|}$.

For illustration consider the graphs in (a) divided by their symmetry factors in (b) to $O(\kappa^3)$:

$W_\kappa[H] \overset{(a),(b)}{=}$  (84)

Upon application of parts (c),(d) this matches the recursively computed result. Generally, the graph rule can be recast symbolically as:

$$W_l[H] = \sum_{C=(V,E)\in\mathcal{C}_l} \frac{(-)^l}{\mathrm{Sym}(C)} \prod_{e\in E} \ell_{\theta(e)} \prod_{v\in V} \omega_{d(v)}(H_v)\,, \tag{85}$$

where the lattice summations from step (d) are tacit and the double product comprises $\mu^W(C)$. The graph sum is over all connected graphs $C = (V, E)$ with $|E| = l$ edges, $d(v)$ is

the degree of the vertex v, $\theta(e)$ is the pair of vertices $e \in E$ connects. A recent algorithm that generates these graphs can be found in [72]. The symmetry factor $\mathrm{Sym}(C)$ of C is defined below. Since also the graph terminology is not entirely standardized we compiled a brief glossary at the end of this subsection.

Once $W[H]$ is known to some order, the connected correlation functions (or cumulants) can be obtained by differentiation. It is plain from (85) that the cumulants $(W^{(k)}[H])_{y_1,\ldots,y_k}$, $y_1 \neq \ldots \neq y_k$, also have a graph expansion and that the contributing graphs are k-rooted, i.e. have k external vertices eventually labeled by $y_1, \ldots, y_k$. The relevant symmetry factor thus is that of the k-rooted graph, where the isomorphisms have to leave the external vertices individually invariant. The edges are assigned a $-\ell_{ij}$ factor as before, also for edges where one of the vertices is an external vertex. The vertex weight can always be obtained by differentiation from the $\omega_{d(v)}(H_v)$ product in (85).

A brief graph glossary:

A *graph* is a pair $G = (V, E)$ of nonempty disjoint sets equipped with a map θ that associates to each $e \in E$ an unordered pair $\theta(e) = \{v, w\}$, $v, w \in V$. The elements of V are called vertices (or nodes), those of E are called edges (or links, or lines). This definition allows for several edges to be mapped into the same unordered pair of vertices, in which case the edges are called multiple edges. Otherwise the graph is called simple, in which case we shall identify E with a subset of $V_2 := \big\{\{v, w\} : v, w \in V\big\}$. The degree (or valency or number of incident lines) $d(v)$ of a vertex $v \in V$ is the cardinality of the set $\{e \in E : v \in \theta(e)\}$. If $|V|_k$ is the cardinality of $\{v \in V : d(v) = k\}$ one has $2|E| = \sum_k k|V|_k$.

Let (V, E) be a graph. A *trail* from v to w, $v, w \in V$ is a sequence $v_0, e_1, \ldots, e_n, v_n$ with $v_0 = v$, $v_n = w$, such that the edges e_i are distinct and $\theta(e_i) = \{v_{i-1}, v_i\}$. A graph is connected if for every pair of its vertices v, w there is a trail from v to w. A connected component of G is a maximal connected subgraph of G. A trail from v to w such that v and w coincide is called a cycle. The cyclomatic number $c(G)$ is the number of cycles of a graph G. The Euler relation states

$$c(G) = |E| - |V| + 1\,. \tag{86}$$

A *tree* T is a connected simple graph without cycles; in particular $|V| - |E| = 1$ holds.

Two graphs (V, E) and (V', E'), with respective maps θ, θ', are called isomorphic (or

topologically equivalent) if there exist bijections $\pi_1 : V \to V'$, $\pi_2 : E \to E'$ such that $\theta(e) = \{v, w\}$ *iff* $\theta'(\pi_2(e)) = \{\pi_1(v), \pi_1(w)\}$. These isometries form a group, $\mathrm{Aut}(G)$, which with the above definition included permutations of multiple edges. The *symmetry factor* of G is defined by

$$\mathrm{Sym}(G) = |\mathrm{Aut}(G)| \,. \tag{87}$$

Often the automorphism group refers to the corresponding simple graph only, in which case the permutation of multiple edges occurs as an extra factor in the definition of the symmetry factor [105, 85].

The same notion of isometry applies if the elements of a subset $R \subset V$, called the rooted vertices, are left individually invariant by the bijection. The elements of R can be viewed as distinguishable and labeled, $R = \{r_1, \ldots, r_k\}$, in which case G is called k-rooted.

A graph $G' = (V', E')$ is called a subgraph of $G = (V, E)$ if $V' \subset V$ and $E' \subset E$. For a graph G let $G\backslash\{v\}$ be the subgraph obtained by deleting v and all edges containing v. For a connected graph $G = (V, E)$ a vertex $v \in V$ is called an *articulation point* if the $G\backslash\{v\}$ is disconnected. A connected graph without articulation points is called one-vertex irreducible (**1VI**) (or two-connected). For a connected graph G a *block* G' is a maximal 1VI subgraph, i.e. a graph $G' \subset G$ that is 1VI and such that for any 1VI subgraph G'' the inclusion $G' \subset G'' \subset G$ entails $G'' = G'$. The set of blocks $\{G_1, \ldots, G_k\}$, $G_i = (V_i, E_i)$, $i = 1, \ldots, k$, of a connected graph $G = (V, E)$ is referred to as G's block decomposition [54]. The blocks induce a partition of the edge set $E = E_1 \cup \ldots \cup E_k$, with $E_i \cap E_j = \emptyset$, $i \neq j$. Each articulation point belongs to more than one V_i while non-articulation vertices belong to exactly one.

A bridge in a connected graph is an edge whose omission produces a disconnected graph. A one-line irreducible (**1LI**) graph is a bridgeless connected graph. A one-line irreducible graph may still get disconnected upon removal of a vertex. The block decomposition of 1LI graphs will be central later on.

3.2.2 The role of one-line and one-vertex irreducible graphs

Our task will be to convert the above W-graph rules into ones directly applicable to the Γ_κ expansion defined by (79). Both functionals are related by the following modified Legendre transform

$$\Gamma_\kappa[\phi] := \phi \cdot H_\kappa[\phi] - W_\kappa[H_\kappa[\phi]] - \kappa\mathcal{V}[\phi]\,, \quad \frac{\delta W_\kappa}{\delta H}\big(H_\kappa[\phi]\big) = \phi\,, \tag{88}$$

for a κ-independent mean field ϕ. The modification by the $\mathcal{V}[\phi] := \frac{1}{2}\sum_{x,y}\phi_x\ell_{xy}\phi_y$ term is introduced so as to obtain the closed flow equation (79). Differentiating (88) with respect to κ gives $\partial_\kappa\Gamma_\kappa = -(\partial_\kappa W_\kappa)[H_\kappa[\phi]] - \mathcal{V}[\phi]$. Inserting the series expansions

$$\begin{aligned} W_\kappa[H] &= \sum_{l\geq 0}\kappa^l W_l[H]\,, \quad \Gamma_\kappa[\phi] = \sum_{l\geq 0}\kappa^l\Gamma_l[\phi]\,, \;\; \Gamma_1[\phi]\equiv 0\,, \\ H_\kappa[\phi] &= \sum_{l\geq 0}\kappa^l H_l[\phi]\,, \qquad H_l = \Gamma_l^{(1)} + \delta_{l,1}\mathcal{V}^{(1)}\,, \;\; l\geq 0\,, \end{aligned} \tag{89}$$

one obtains $\Gamma_0[\phi] = \phi\cdot H_0[\phi] - W_0[H_0[\phi]]$, $\Gamma_1[\phi] = -W_1[H_0[\phi]] - \mathcal{V}[\phi]\equiv 0$, and for $l\geq 2$

$$\Gamma_l[\phi] = -W_l[H_0[\phi]] - \sum_{m=1}^{l-1}\sum_{k=1}^{m}\frac{l-m}{lk!}\sum_{\substack{m_1+\ldots+m_k=m\\ m_j\geq 1}} W_{l-m}^{(k)}[H_0[\phi]]\cdot H_{m_1}[\phi]\ldots H_{m_k}[\phi]\,. \tag{90}$$

Note that $W_\kappa^{(1)}[H_\kappa[\phi]] = \phi$ still enters (90) implicitly in defining the $H_m[\phi]$. Upon expansion one finds $W_0^{(1)}[H_0[\phi]] = \phi$, $W_0^{(2)}[H_0[\phi]]\cdot H_1[\phi] + W_1^{(1)}[H_0[\phi]] = 0$, and for $l\geq 2$

$$H_l[\phi]\cdot W_0^{(2)}[H_0[\phi]] + W_l^{(1)}[H_0[\phi]] + \frac{\delta}{\delta H_0}F_{l-1}[H_0,H_1,\ldots,H_{l-1}]\Big|_{H_m=H_m[\phi]} = 0\,, \tag{91}$$

where

$$\begin{aligned} F_{l-1}[H_0,\ldots,H_{l-1}] &:= \sum_{m=1}^{l-1}\sum_{k=1}^{m}\check{B}_{mk}(H_1,\ldots,H_{m-k+1})\cdot W_{l-m}^{(k)}[H_0] \\ &\quad + \sum_{k=2}^{l}\check{B}_{lk}(H_1,\ldots,H_{l+1-k})\cdot W_0^{(k)}[H_0]\,, \end{aligned} \tag{92}$$

and the $\check{B}_{m,k}$ are modified Bell polynomials, $k!\check{B}_{mk}(H_1,\ldots,H_{l-k+1}) := \sum_{m_1+\ldots+m_k=m,m_j\geq 1} H_{m_1}H_{m_2}\ldots H_{m_k}$. These relations can be solved iteratively for the $H_l[\phi]$ and also show inductively that $H_l[\phi] = \Gamma_l^{(1)}[\phi]$.

In (90), (91) and similar relations later on there are tacit summations over lattice sites, summarily indicated by a "$\cdot$". A contraction of $(W^{(k)}_{l-m})_{y_1 \dots y_k}$ may contain subsums where where one or more lattice points coincide. The graph rules for the cumulants outlined after (85) then change slightly. Since multiple h derivatives can act on the same $\omega_{d(v)}(h)$, the number of rooted vertices r can be $r = 1, \dots, k$. The tacit lattice sums ensure that all possible combinations will occur, so that $W^{(k)}_{l-m}$ expands into a sum of r-rooted connected graphs with $l-m$ edges; we write $\mathcal{C}^{\bullet r}_{l-m}$ for the set of such graphs. The topology of each graph in $\mathcal{C}^{\bullet r}_{l-m}$ is the same as its counterpart in $\mathcal{C}_{l-m}$, only the rooted vertices have their ω_n weight shifted from $n = d(v)$ to $n = d(v) + \#$of h-derivatives, and the symmetry factor changes. The contracted lattice sums in (90), (91) ensure that each graph in $\mathcal{C}^{\bullet r}_{l-m}$ is paired with an r-rooted product of $H_{m_1}, \dots, H_{m_k}$'s graph expansions, such that a term corresponding to an unrooted $\mathcal{C}_l$ graph arises. This graph expansion of (90)'s right hand side allows for many cancellations. In order to identify the underlying pattern we derive a property of the LRH expansion of the effective action well-known for its perturbative expansion but not limited to it:

Lemma 3.2.1. *The graphs contributing to $\Gamma_\kappa[\phi]$'s LRH expansion are 1LI, i.e. remain ℓ-connected even when any one ℓ-line is cut.*

Proof. The proof is an adaptation of the argument familiar for the Feynman diagrams occurring in a perturbative expansion. In a first step one computes the linear response of $\Gamma_\kappa[\phi]$ under a replacement of the hopping matrix

$$\ell_{xy} \mapsto \ell_{xy} + \epsilon e_x e_y \,, \tag{93}$$

where e_x is a vector and $\epsilon \geq 0$. We momentarily change notation and write $W_\epsilon[H]$, $\Gamma_\epsilon[\phi]$ for the functionals obtained by the replacement (93) and $W[H], \Gamma[\phi]$ for the original ones, without indicating the κ-dependence. Starting from the functional integral realization

$$\begin{aligned} &\exp W[H] := \int \prod_x d\chi_x \exp\{-S[\chi] + \sum_x H_x \chi_x\} \,. \\ &S[\chi] = S_0[\chi] + \kappa \mathcal{V}[\chi] \,, \quad S_0[\chi] = \sum_x s(\chi_x) \,, \quad \mathcal{V}[\chi] = \frac{1}{2} \sum_{x,y} \chi_x \ell_{xy} \chi_y \,. \end{aligned} \tag{94}$$

and expanding in powers of ϵ one finds to linear order

$$W_\epsilon[H] = W[H] - \epsilon\frac{\kappa}{2}\sum_{x,y} e_x e_y \left(\frac{\delta^2 W}{\delta H_x \delta H_y} + \frac{\delta W}{\delta H_x}\frac{\delta W}{\delta H_y}\right) + O(\epsilon^2)\,. \tag{95}$$

For the altered functionals the definition of the modified Legendre transform (88) reads

$$\Gamma_\epsilon[\phi] = \phi\cdot H_\epsilon[\phi] - W_\epsilon[H_\epsilon[\phi]] - \frac{\kappa}{2}\phi\cdot(\ell + \epsilon e\otimes e)\cdot\phi\,, \quad \frac{\delta W_\epsilon}{\delta H}\big(H_\epsilon[\phi]\big) = \phi\,. \tag{96}$$

Differentiating with respect to ϵ gives $\partial_\epsilon\Gamma_\epsilon[\phi] = \frac{\kappa}{2}(e\otimes e)W^{(2)}(H[\phi]) + O(\epsilon)$. Since $W^{(2)}(H[\phi]) = (\Gamma^{(2)} + \kappa v)^{-1}$ one obtains

$$\Gamma_\epsilon[\phi] = \Gamma[\phi] + \epsilon\frac{\kappa}{2}\sum_{x,y} e_x e_y \big[\Gamma^{(2)} + \kappa\ell\big]^{-1}_{xy} + O(\epsilon^2)\,. \tag{97}$$

The replacement (93) emulates the effect of cutting ℓ-lines and to linear order in ϵ the effect of cutting precisely one ℓ-line is traced. Viewed as a function of H the response, being proportional to $W^{(2)}[H]$, expands into ℓ-connected LRH graphs by Section 3.2.1. The recursion (91) shows that the κ expansion of $H[\phi]$ produces contracted functional derivatives of the $W_0, W_1, \ldots, W_l$ evaluated at $H_0[\phi]$ for all $H_l[\phi]$, $l \geq 1$. The $W_m^{(k)}$ derivatives correspond to $r \leq k$-rooted ℓ-connected diagrams and the contractions are pointwise with analogous terms. Hence, also as a functional of ϕ the linear response (97) expands into ℓ-connected LRH graphs only. □

The graph expansion of the right hand of (90) contains a large number of terms associated with one-line reducible graphs. By Lemma 3.2.1 these must cancel which allows one to simplify the right hand side considerably. In the sum each $W_{l-m}^{(k)}$ expands into r-rooted, $r = 1, \ldots, k$, connected diagrams many of which are one-line reducible. The rooted vertices are directly (without extra ℓ_{xy} link) attached to (and summed over the lattice point associated with) possibly multiple copies of a 1-rooted graph representing a $\Gamma_m^{(1)} + \delta_{m,1}\mathcal{V}^{(1)}$. A term occurring in the graph expansion of $W_{l-m}^{(k)}[H_0[\phi]]\cdot H_{m_1}[\phi]\ldots H_{m_k}[\phi]$ will be one-line reducible if (i) $m_i = 1$ for one or more $i \in \{1, \ldots, k\}$, since $H_1[\phi]_x = \sum_y \ell_{xy}\phi_y$. (ii) the r-rooted W-graph stemming from $W_{l-m}^{(k)}$ is one-line reducible. (iii) if a $W_1^{(k)}$ term enters, as $W_1[H] = -\frac{1}{2}\sum_{x,y}\ell_{xy}\omega_1(H_x)\omega_1(H_y)$. All these terms must cancel against the one-line reducible terms in $-W_l$. We write $W_l^{(k)}[\Gamma_0^{(1)}]|_{1\mathrm{LI}}$ for the quantity obtained from $W_l^{(k)}[\Gamma_0^{(1)}]$'s graph expansion

by omitting all terms corresponding to one-line reducible graphs and $[m]$ for the integer part of $m \in \mathbb{R}_+$. Then $\Gamma_2[\phi] = -W_2[\Gamma_0^{(1)}]|_{1\mathrm{LI}}$, $\Gamma_3[\phi] = -W_3[\Gamma_0^{(1)}]|_{1\mathrm{LI}}$, and for $l \geq 4$ the following simplified version of (90) holds

$$\Gamma_l[\phi] = -W_l[\Gamma_0^{(1)}]\Big|_{1\mathrm{LI}} - \sum_{m=2}^{l-2} \sum_{k=1}^{[m/2]} \sum_{\substack{m_1 + \ldots + m_k = m \\ m_i \geq 2}} \frac{(l-m)}{lk!} W_{l-m}^{(k)}[\Gamma_0^{(1)}]\Big|_{1\mathrm{LI}} \cdot \Gamma_{m_1}^{(1)} \ldots \Gamma_{m_k}^{(1)} . \tag{98}$$

An immediate consequence of (98) is:

Lemma 3.2.2. *Let L be a 1LI graph without articulation points and let $\mu^W(L), \mu^\Gamma(L)$ be the weight (including sign and symmetry factors) with which it occurs in the expansion of W, Γ, respectively. Then*

$$\mu^\Gamma(L) = -\mu^W(L)\big|_{H_0 = \Gamma_0^{(1)}} . \tag{99}$$

Proof. It suffices to show that all terms in the sum on the right hand side of (98) expand into graphs with articulation points. As seen above, each $W_{l-m}^{(k)}|_{1\mathrm{LI}}$ expands into r-rooted, $r = 1, \ldots, k$, 1LI graphs that are directly (without extra ℓ_{xy} link) attached to an r-rooted product $\Gamma_{m_1}^{(1)} \ldots \Gamma_{m_k}^{(1)}$ (with the same $\Gamma_m^{(1)}, m \geq 2$, possibly occurring several times) where each factor expands into 1-rooted 1LI graphs. Each of the rooted vertices therefore is an articulation point and the graphs contributing to a $W_{l-m}^{(k)}|_{1\mathrm{LI}}$ term in the sum have at least one articulation point. □

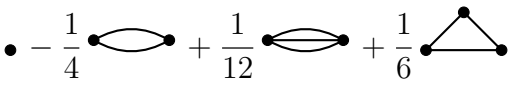
On account of the previous results the problem of finding a graph rule for the LRH expansion of Γ_κ has been reduced to understanding the weight $\mu^\Gamma(v)$ that ought to be assigned to articulation points: by Lemma 3.2.1 we know that the graphs contributing to $\Gamma_l[\phi]$ are one-line irreducible (1LI). As long as the 1LI graph considered has no articulation points Lemma 3.2.2 straightforwardly provides the weight. The same reasoning shows that the maximal number of articulation vertices in some $L \in \mathcal{L}_l$ is $[(l-2)/2]$. One may anticipate a trade-off to occur: the vastly reduced number of graphs to be considered (compared to W) will be compensated in part by a more complicated weight assignment for articulation vertices. Overall a very significant simplification is found to occur already at low orders; see

Table 2 [1].

l	$\lvert\mathcal{C}_l\rvert$	$\lvert\mathcal{L}_l\rvert$	# art. vert.
3	5	2	0
4	12	4	1
5	33	8	2
6	101	22	8,1

Table 2: Number of connected, one-line irreducible, one-line irreducible graphs with $1, 2, \ldots$ articulation points, respectively, and l edges.

Up to $l = 3$ all 1LI graphs are also 1VI, so that the graph rules for W_l (with vertex weights $\omega_m(\varphi) := \omega_m(h)|_{h=h(\varphi)}$, $m \geq 1$) gives the correct answer for $l \leq 3$. In the figure below the weights from the W rule match the terms in the directly computed result (513):

$\Gamma[\phi]$ =  $+ O(\kappa^4)$. (100)

For $l = 4$ the same works for all but the second to last term, which corresponds to a "pair of glasses" graph. The vertex in the middle is an articulation point and by inspection of (513) one reads off the weight that should be attributed to it:

Symmetry factor $= 2^3$

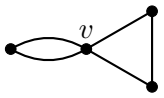
$$\mu^\Gamma(v) = \omega_4(\varphi_v) - \gamma_2(\varphi_v)\omega_3(\varphi_v)^2\,. \tag{101}$$

In each case we also note the symmetry factor of the full graph next to it. For $l = 5$ there are two graphs with articulation points for which the explicitly computed weights are:

Symmetry factor $= 2 \times 3!$

$$\mu^\Gamma(v) = \omega_5(\varphi_v) - \gamma_2(\varphi_v)\omega_3(\varphi_v)\omega_4(\varphi_v)\,. \tag{102}$$

[1] $|\mathcal{C}_6| = 101$ corrects a typo in the published version.



Symmetry factor $= 2^2$

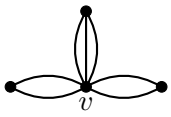
$$\mu^{\Gamma}(v) = \omega_4(\varphi_v) - \gamma_2(\varphi_v)\omega_3(\varphi_v)^2\,. \tag{103}$$

Clearly, the first term in the weight associated to an articulation point is the one expected from the W graph rules; it is the systematics of the additional terms that need to be understood.

3.2.3 Recursive computation of the weights of articulation points

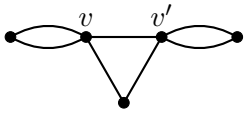
Our guiding principle in pinning down these systematics will be the relation (98). It expresses Γ_l's graph expansion in terms of those of $\Gamma_2^{(1)}, \ldots, \Gamma_{l-2}^{(1)}$, modulo pieces known from the W-graph rules. By construction (98) is equivalent to the closed recursion (511). In contrast to (511) the mixed recursion (98) allows one to isolate directly contributions from individual graphs, in particular those with articulation points. For example, for $l=4$ one has $\Gamma_4 = -W_4|_{1\mathrm{LI}} - \frac{1}{2}W_2^{(1)}|_{1\mathrm{LI}} \cdot \Gamma_2^{(1)}$. Applying the graphical differentiation rules to W_2 and Γ_2 one quickly recovers (101). Similarly, for $l = 5$ one obtains from (98) $\Gamma_5 = -W_5|_{1\mathrm{LI}} - \frac{3}{5}W_3^{(1)}|_{1\mathrm{LI}} \cdot \Gamma_2^{(1)} - \frac{2}{5}W_2^{(1)}|_{1\mathrm{LI}} \cdot \Gamma_3^{(1)}$, and (102), (103) can be confirmed graphically. With Γ_l, $l = 2, \ldots, 5$, known explicitly from Appendix A the same procedure allows one to obtain the weights of all $l = 6, 7$ graphs with articulation points. At $l = 6$ there are 8 graphs with one articulation vertex and 1 with two articulation vertices, see Table 1. The $l = 6$ graph with two articulation vertices is the "triple bubble" graph and both have the same weight associated to them as v in (101).

More interesting are the $l = 7$ graphs for which we present three examples:



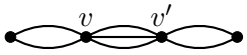
Symmetry factor $= 2^3 \times 3!$

$$\mu^{\Gamma}(v) = \omega_7 - 2\gamma_2\omega_3\omega_6 - \gamma_2\omega_4\omega_5 + \gamma_2^2\omega_3^2\omega_5 + 2\gamma_2^2\omega_3\omega_4^2 + \gamma_3\omega_3^2\omega_4 \tag{104}$$



Symmetry factor $= 2^3$

$$\mu^{\Gamma}(v) = \mu^{\Gamma}(v') = \omega_4 - \gamma_2\omega_3^2 \tag{105}$$

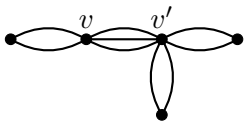


$$\text{Symmetry factor} = 2^3 \times 3!$$

$$\mu^\Gamma(v) = \mu^\Gamma(v') = \omega_5 - \gamma_2\omega_3\omega_4 \tag{106}$$

Here and below we omit the φ arguments of the ω_m's. Note that the weight in (104) is new while those in (105) and (106) are recycled from (101), (103) and (102), respectively.

So far the graph expansion of the explicitly computed $\Gamma_2, \dots, \Gamma_5$ from Appendix A could be used as an input to obtain the results for all $l = 6, 7$ graphs. The recursion (98) also allows one compute the weights of individual higher order graphs *without* knowing the full results for the Γ_m's at lower orders. We illustrate this with two $l = 9$ graphs chosen so that the $l = 7$ input graphs are among the ones preciously displayed.

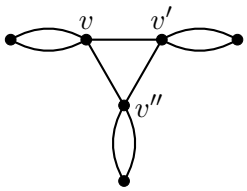


$$\text{Symmetry factor} = 2^4 \times 3!\,; \;\; \text{input } (104), (106)$$

$$\mu^\Gamma(v) = \omega_5 - \gamma_2\omega_3\omega_4$$

$$\mu^\Gamma(v') = \omega_7 - 2\gamma_2\omega_3\omega_6 - \gamma_2\omega_4\omega_5 \tag{107}$$

$$+ \gamma_2^2\omega_3^2\omega_5 + 2\gamma_2^2\omega_3\omega_4^2 + \gamma_3\omega_3^2\omega_4$$



$$\text{Symmetry factor} = 2^3 \times 3!\,; \;\; \text{input } (105)$$

$$\mu^\Gamma(v) = \mu^\Gamma(v') = \mu^\Gamma(v'') = \omega_4 - \gamma_2\omega_3^2\,. \tag{108}$$

These examples illustrate a pattern that holds generally. To formulate it we introduce a natural grading for the quantities considered. It is induced by the derivatives of the single site functions $\omega(h), \gamma(\varphi)$ and their interrelations discussed in Appendix B.

Lemma 3.2.3. *For a monomial in $\omega_m, m \geq 3$, ω_2^{-1}, define its degree by:* $\deg \omega_m = m, \deg \omega_2^{-1} = -2$*, and extended additively to products. Then:*

(a) $\deg\gamma_m = -m$, $m \geq 2$.

(b) $\deg W_l^{(k)} = 2l+k$, $\deg\Gamma_l^{(k)} = 2l-k$, $k \geq 0$, *to all orders* $l \geq 1$ *of the LRH expansion.*

(c) The weight $\mu^\Gamma(v)$ *assigned to an articulation vertex* v *has homogeneous degree* $\deg[\mu^\Gamma(v)]$ *which coincides with its degree in the* W*-graph rule, i.e.* $\deg[\mu^W(v)] = l$*, for an* l*-valent vertex.*

(d) The weight $\mu^\Gamma(v)$ *assigned to an articulation vertex* v *of degree* $d(v) = m \geq 4$ *can be normalized such that*

$$\mu^\Gamma(v) = \omega_m - \sum_{3i_3+\ldots+(m-1)i_{m-1}=m+2i_2} d_{i_3\ldots i_{m-1}} (\omega_2^{-1})^{i_2} \omega_3^{i_3} \ldots \omega_{m-1}^{i_{m-1}}\,, \tag{109}$$

and analogously in any mixed ω_m, γ_m *form.*

Proof. (a) Manifest from (518). (b) $W_1[H] = -\frac{1}{2}\sum_{x,y} \ell_{xy}\omega_1(H_x)\omega_1(H_y)$ gives $\deg W_1 = 2$, each H derivative raises the degree by 1, so $\deg W_l = 2l$ follows from the recursion (82). Similarly, $\deg\Gamma_2 = 4$ from (513), each ϕ derivative lowers the degree by 1 (as $\partial_\varphi = \gamma_2\partial_h$), and $\deg\Gamma_l = 2l$ follows from the recursion (511). Since $\deg W_{l-m}^{(k)} = 2(l-m)+k$, $\deg[\Gamma_{m_1}^{(1)} \ldots \Gamma_{m_k}^{(1)}] = 2(m_1+\ldots+m_k)-k$, compatibility with (90) is ensured. (c) The weight $\mu^\Gamma(v)$ is in principle determined by the recursion (90), (98). By (b) these relations preserve homogeneity which implies $\deg[\mu^\Gamma(v)] = \deg[\mu^W(v)]$. (d) is a consequence of (c) and the gross structure of (98). □

In summary, let $\mathcal{L}_l$ be the set of one-line irreducible graphs with $l = |E|$ links. Then

$$\Gamma_l[\phi] = \sum_{L=(V,E)\in\mathcal{L}_l} \frac{(-)^{l+1}}{\mathrm{Sym}(L)} \prod_{e\in E} \ell_{\theta(e)} \prod_{v\in V} \mu^\Gamma(v|L)\,, \tag{110}$$

with a tacit unconstrained sum over the lattice points associated with the vertices upon embedding. Here $\mu^\Gamma(v|L)$ is as in (109) where only the coefficients $d_{i_3,\ldots,i_{m-1}}$ remain to be determined. These coefficients depend on the 1VI subgraphs that are joined at the articulation vertex, not just on the degree of the vertex; so we write $\mu^\Gamma(v|L)$ from now on.

For completeness' sake we justify in detail why the weights $\mu^\Gamma(v|L)$, $L \in \mathcal{L}_l$, are determined recursively by (98). For the graphical evaluation of (98), graph rules for $\Gamma_m^{(1)}, m = 1,\ldots,l-2$, are needed. Differentiating (110) produces an analogous expansion in terms of

1-rooted one-line irreducible graphs for which we write $\mathcal{L}_m^{\bullet 1}$ at order $|E| = m$. The product over $\mu^\Gamma(v|L)$ extends over all but the rooted vertex, where $\partial\mu^\Gamma/\partial\varphi$ occurs. In the context of (98) the coefficients $d_{i_1\ldots i_{m-1}}$ entering the $\Gamma_m^{(1)}$, $m = 1, \ldots, l-2$, are assumed to be known and those for the graphs in $\mathcal{L}_l$ are to be determined. The additional piece of information entering are the graph rules for $W_{l-m}^{(k)}|_{1\mathrm{LI}}$, $1 \leq k \leq [m/2]$. These can be inferred from (85). Since multiple h derivatives can act on the same $\omega_{d(v)}(h)$, the number of rooted vertices r can be $r = 1, \ldots, k$. The tacit lattice sums ensure that all possible combinations will occur, so that $W_{l-m}^{(k)}|_{1\mathrm{LI}}$ expands into a sum of r-rooted 1LI graphs with $l-m$ edges, the set of which we denote by $\mathcal{L}_{l-m}^{\bullet r}$. The topology of each graph in $\mathcal{L}_{l-m}^{\bullet r}$ is the same as its counterpart in $\mathcal{L}_{l-m}$, only the rooted vertices have their ω_m weight shifted from $m = d(v)$ to $m = d(v) + \#$of h-derivatives, and the symmetry factor changes. Each term in the graph expansion of $W_{l-m}^{(k)}[\Gamma_0^{(1)}]|_{1\mathrm{LI}} \cdot \Gamma_{m_1}^{(1)} \ldots \Gamma_{m_k}^{(1)}$, then has the rooted subgraphs joined at the roots so that an unrooted graph in $\mathcal{L}_l$ arises. In any concrete instance the procedure is evident and has been used to work out the previous examples. The formulation of the general evaluation principle for (98)'s right hand side justifies that the recursion works generally and just needs to be 'solved'.

3.3 Graph implementation of the $\Gamma_\kappa[\phi]$ LRH expansion

So far each Γ_l is known to expand into 1LI irreducible graphs L whose weights in (110) are known modulo the coefficients $d_{i_3,\ldots i_{m-1}}$ in (109). These coefficients depend on the decomposition of L into 1VI subgraphs, turn out to be integers, and can be understood in terms a separate set of *tree* graphs. To preclude a possible confusion let us stress that these tree graphs are conceptually and technically different from the ones governing the interplay between vertex functions and connected correlation functions, see Appendix B for the latter.

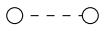
3.3.1 Labeled tree graphs

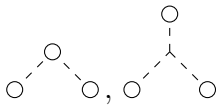
We begin by introducing a class of unlabeled tree graphs called 'dashed', which get labeled in a second step.

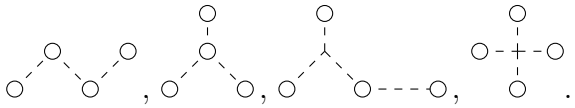
Definition: The 'dashed' graphs are tree graphs where two types of vertices are connected by dashed lines. The set of "open circle" vertices is denoted by ν_0, the set of "dashed" vertices is denoted by ν_1, and the edge list $\epsilon \subset (\nu_0 \cup \nu_1)_2$ is constrained as follows. The valency of an open circle vertex is $1, 2, \ldots$, dashed vertices have valency $3, 4, \ldots$, and no two dashed-vertices are connected by a single dashed line. The Euler relation for tree graphs then holds in the form $|\nu_0| + |\nu_1| = |\epsilon| + 1$. We write $\mathcal{T}_n$ for the set of topologically distinct such graphs with $n = |\nu_0|$ open circle vertices.

For example the graphs in $\mathcal{T}_1, \ldots, \mathcal{T}_4$ are

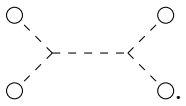
$\mathcal{T}_1$  (111)

$\mathcal{T}_2$ 

$\mathcal{T}_3$ 

$\mathcal{T}_4$ 

The restriction that no two dashed-vertices can be connected by a single dashed line eliminates from consideration graphs of the form



The graphs in $\mathcal{T}_{n+1}$ can be obtained from those in $\mathcal{T}_n$ by adding one dashed leg with an open circle in all topologically inequivalent ways to an open circle, a dashed line, or a dashed vertex. Further, the constituents of a dashed graph can be attributed a "dashed degree

ddeg" as follows:

$$\begin{aligned} &|o|\text{-valent open circle vertex } o,\ |o|\geq 1 \qquad && \text{ddeg} = |o| + d_j\,, \\ &\text{dashed line connecting two open circles} && \text{ddeg} = -2\,, \\ &m\text{-valent dashed vertex, } m\geq 3 && \text{ddeg} = -m\,. \end{aligned} \tag{112}$$

Here $d_j, j = 0, \ldots, n-1$, are integers whose significance will become clear shortly. Then:

$$\text{ddeg}(t) = \sum_{j=0}^{n-1} d_j\,, \quad \text{for any dashed graph } t\in\mathcal{T}_n,\ n\geq 2\,. \tag{113}$$

This can be seen by induction on n using the before mentioned recursive generation. Any of the three operations generating a graph in $\mathcal{T}_{n+1}$ from one in $\mathcal{T}_n$ is readily seen to preserve ddeg. By inspection of (111) the assertion holds for $n = 1, 2, 3$ and (113) follows. Note that this gives a more fine grained invariant than merely the Euler relation (86) for tree graphs. Instead of viewing the d_j as parameterizing the ddeg function one may also regard them as labels for the dashed graphs themselves. We then write $\mathcal{T}_n^D$ for the set of dashed graphs $\mathcal{T}_n$ with an integer from the n-tuple $D = (d_0, d_1, \ldots, d_{n-1})$ assigned to each open circle vertex. The use of an n-tuple is natural in the iteration of the map (115) below. Later on we use the same notation $\mathcal{T}_n^D$ when D is a multiset of integers of cardinality n.

Compatibility with differentiation:

Each $\tau\in\mathcal{T}_n^D$ can be assigned a weight $\mu(\tau)$ as follows

$$\begin{aligned} \omega_{|o|+d_j} \quad &\text{to an } |o|\text{-valent open circle vertex } o,\ |o|\geq 1\,, \\ \gamma_2 \quad &\text{to a dashed line connecting two open circles}\,, \\ \gamma_m \quad &\text{to an } m\text{-valent dashed vertex, } m\geq 3\,. \end{aligned} \tag{114}$$

The degree of each factor in $\mu(\tau)$ equals the ddeg of the underlying graph, $d(\omega_{|o|+d_j}) = |o| + d_j = \text{ddeg}(|o|\text{-valent open circle vertex})$, etc. Hence $d(\mu(\tau)) = \sum_{j=0}^{n-1} d_j$, for all $\tau\in\mathcal{T}_n^D$. We write $\mu(\mathcal{T}_n^D)$ for the span of all $\mu(\tau), \tau\in\mathcal{T}_n^D$. Augmenting a $(n+1)$-st integer d_n we claim that

$$\omega_{d_n+1}(\varphi)\partial_\varphi : \mu(\mathcal{T}_n^D)\to\mu(\mathcal{T}_{n+1}^D)\,, \tag{115}$$

with the understanding that $D = (d_0, \ldots d_{n-1}, d_n)$ in the range. This follows from the basic

differentiation rules $\partial_\varphi \omega_m = \gamma_2 \omega_{m+1}$, $\partial_\varphi \gamma_m = \gamma_{m+1}$ and the way $\omega_{d_n+1}\partial_\varphi$ acts on the three types of factors in each $\mu(\tau)$: acting on ω_{d_j+1} the operator produces $\omega_{d_n+1}\gamma_2\omega_{d_j+1}$, equivalent to adding a dashed edge with an open circle vertex to an existing open circle vertex. Acting on γ_2 it produces $\omega_{d_j+1}\gamma_3$, which adds a dashed edge with an open circle to a dashed line. Finally, acting on γ_m, $m \geq 3$, gives $\omega_{d_j+1}\gamma_{m+1}$, which adds a line with an open circle to an existing dashed vertex. These basic operations are in one-to-one correspondence to those generating the unlabeled graphs $\mathcal{T}_{n+1}$ from $\mathcal{T}_n$, verifying that (115) has the correct range. Starting at $n = 1$ with an ω_{d_0} assigned to the open circle vertex, one may verify directly that repeated action of (115) produces a sum of terms whose underlying graphs match those in (111) but with integers $|o| + d_j$, $j = 0, 1, 2 \ldots$, assigned to their open circle vertices. The map (115) provides the raison d'être for the dashed graphs.

Lemma 3.3.1. *The recursion (98) generates only vertex weights $\mu^\Gamma(v|L)$ in (110) that lie in the (v-dependent) direct sum of $\mu(\mathcal{T}_n^D)$, for $n = 1, \ldots, n_{\max}$, $n_{\max} \leq d(v) - 3$, for some integer multiset D_n.*

Proof. We proceed by induction on l with $L \in \mathcal{L}_l$. The assertion holds by inspection of (101), (102), (103) for $l = 4, 5$. For the $l - 1 \mapsto l$ step in the recursion (98) we denote by $L_j \in \mathcal{L}_{m_j}$ one of the 1LI graphs in Γ_{m_j}'s graph expansion and by $L^W \in \mathcal{L}_{l-m}$ one of the 1LI graphs in W_{l-m}'s expansion. We focus on one of the vertices v where the graphs are joined and write v_0 for v's copy in L^W and v_j for v's copy in L_j^Γ, $j = 1, \ldots, k$. By the W-graph rule the structure of L^W is irrelevant only the weight $\omega_{d(v_0)}(h)|_{h=H_v}$ (and the inverse symmetric factor $\mathrm{Sym}(L^W)$ irrelevant here) enters. If r of the k functional differentiations with respect to some H_i act on the chosen H_v site the weight will be shifted to $\omega_{d(v_0)+r}(h)|_{h=h(\varphi_v)}$. The associated graph will still be denoted by L^W; it now has one rooted vertex v_0 to which we attribute multiplicity r. The single differentiation of Γ_{m_j} with respect to some ϕ_i will always produce 1-rooted graphs, and for the ones rooted at v_j we write $L_j^\Gamma \in \mathcal{L}_{m_j}^{1\bullet}$. In any one term contributing to (98) at v, a v_0 of multiplicity r will have r 1LI graphs attached, which are selected from the $L_j^\Gamma \in \mathcal{L}_{m_j}^{1\bullet}$, $j = 1, \ldots, k$. Without loss of generality we take $L_j^\Gamma \in \mathcal{L}_{m_j}^{1\bullet}$, $j = 1, \ldots, r$, as the graphs attached to v_0. For fixed r the weight associated with v is by

(110)

$$\omega_{d(v_0)+r} \prod_{j=1}^{r} \partial_\varphi \mu^\Gamma(v_j|L_j)\,. \tag{116}$$

By the induction hypothesis all $\mu^\Gamma(v_j|L_j)$ have an expansion in the (v_j-dependent) direct sum of $\mu(\mathcal{T}_n^D), n = 1, \ldots, n_{\max}$. Focus on a term with n_j open circle vertices in $\mu^\Gamma(v_j|L_j)$. For $r = 1$ the product (116) is directly of the form (115) and the assertion follows. For $r \geq 2$ one notices that each $\partial_\varphi \mu^\Gamma(v_j|L_j)$ has one degree lower and can be attributed to tree graphs with n_j open circle vertices and an extra edge without open circle (so that these trees are not dashed graphs as defined above). The product (116) contains $1+n_1+\ldots+n_r$ ω_m factors and expands into terms that can again be attributed to dashed graphs. This is because the extra r dashed edges are joined at the extra open circle vertex associated with $\omega_{d(v_0)+r}$. In other words, the set of dashed graphs is closed under a gluing operation that first creates an external dashed edge and then joins any number of such trees at an extra open circle vertex. As $1 \leq r \leq k \leq [m/2]$ runs through all possible values allowed by (98) only terms that can be associated with dashed graphs $\mathcal{T}_n^D$, for some n are generated. Comparison with (109) shows that the maximal n that can occur in a normalized weight $\mu^\Gamma(v|L)$ is $n_{\max} \leq d(v) - 3$ (while the actual $n_{\max}$ turns out to be much smaller). □

It remains to understand the coefficients with which the various dashed graphs occur in $\mu^\Gamma(v|L)$. To this end a different type of labeling turns out to be useful.

Assignment of labels:

The labels are set partitions of vertices as frequently used in other contexts. In the situation at hand, the vertex set $\{b_1, \ldots, b_I\}$ will later be identified with the one associated with an articulation vertex v in the block decomposition (as defined at the end of Section 3.2.1) of the underlying one-line irreducible graph L. For now we ignore the origin of the set $B = \{b_1, \ldots, b_I\}$ and consider its set partitions. If all elements of B are distinct, a set partition of B is a set of non-empty disjoint subsets of B whose union is B. An element of a partition is called a cell; we write $\mathcal{S}(B, k)$ for the set partitions of B with k cells. The number of partitions of a set B with I distinct elements into n cells is given by $S(I, n)$, the Stirling number of the second kind. The total number of set partitions is given by the Bell number $B(I) = \sum_{n=1}^{I} S(I, n)$. A convenient generating function is $\exp\{y(e^x - 1)\} =$

$\sum_{I,n\geq 0} S(I,n)\, y^n x^I/I!$. Generalizations have been considered in [33].

The same concept applies to multisets, i.e. sets of pairs (b_i, m_i) where $m_i \in \mathbb{N}$, specifies the multiplicity with which b_i occurs. We write

$$B = \{b_1^{m_1}, \ldots, b_J^{m_J}\} = \{b_i : i \in I\}\,, \quad I = \{\underbrace{1, ..., 1}_{m_1}, \ldots, \underbrace{J, ..., J}_{m_J}\}\,, \tag{117}$$

for the multiset with multiplicities $(m_1, \ldots, m_J) \in \mathbb{N}^J$. In the alternative notation with explicitly repeated elements the indexing I is viewed as a multiset. Two multisets are identical iff they contain the same elements with the same multiplicities. The partitions of a multiset are defined as the set partitions of a $|I| = \sum_j m_j$ element set where m_j copies of b_j are identified afterwards and 'duplicates' are omitted from the list. There are several notions of 'duplicates' one can use; we allow both repeated cells and repeated elements within a cell but eliminate duplicates of the same partition. For example, $\mathcal{S}(\{a, b, c^2\}, 3)$ has 4 elements, $\{\{a\}, \{b\}, \{c^2\}\}$, $\{\{a\}, \{b, c\}, \{c\}\}$, $\{\{a, b\}, \{c\}, \{c\}\}$, $\{\{a, c\}, \{b\}, \{c\}\}$, as opposed to $|\mathcal{S}(\{a, b, c, d\}, 3)| = 6$.

Unless specified otherwise we allow B in the following to be a multiset of the form (117). A partition of B with n cells is then used to label the open circle vertices of a graph in $\mathcal{T}_n$. One may think of each open circle vertex as a 'bag' that contains a cell. Technically, the labeling map is for each partition $\pi \in \mathcal{S}(B, n)$, a bijection $\nu_0 \mapsto \nu_0^\pi$, of sets of cardinality n. While the vertices ν_0 of the unlabeled graph may be assigned 'dummy' labels that can be freely permuted in probing for isomorphisms the elements of ν_0^π can only be permuted if their labels coincide. Isomorphic labeled graphs are defined as in Section 3.2.1, with $V = \nu_0^\pi$ as vertex set. We write $\mathcal{T}(B, n)$, $1 \leq n \leq I$, for the set of topologically inequivalent dashed graphs with n open circle vertices labeled by $\mathcal{S}(B, n)$. Further, for some unlabeled $t \in \mathcal{T}_n$ we write $T \in \mathcal{T}(B, n)$ for one of its labeled counterparts.

As an illustration consider $n = 3$. The set partitions of $B = \{b_1, b_2, b_3\}$ are

$$\begin{aligned}
&\Big\{\{b_1, b_2, b_3\}\Big\},\\
&\Big\{\{b_1\}, \{b_2, b_3\}\Big\},\ \Big\{\{b_2\}, \{b_1, b_3\}\Big\},\ \Big\{\{b_3\}, \{b_1, b_2\}\Big\},\\
&\Big\{\{b_1\}, \{b_2\}, \{b_3\}\Big\}\,.
\end{aligned} \tag{118}$$

These are then assigned as labels to the open circle vertices of the graphs in $\mathcal{T}_1, \mathcal{T}_2, \mathcal{T}_3$:

$$\{b_1, b_2, b_3\} \in \circ$$

$$\{b_1\} \in \circ\text{- - -}\circ \ni \{b_2, b_3\}\,, \quad \{b_2\} \in \circ\text{- - -}\circ \ni \{b_1, b_3\}\,, \quad \{b_3\} \in \circ\text{- - -}\circ \ni \{b_1, b_2\}\,,$$

$$\overset{\{b_2\}}{\{b_1\} \in \circ\!\!\circ \ni \{b_3\}}\,, \qquad \overset{\{b_1\}}{\{b_2\} \in \circ\!\!\circ \ni \{b_3\}}\,, \qquad \overset{\{b_3\}}{\{b_1\} \in \circ\!\!\circ \ni \{b_2\}}\,,$$

$$\overset{\{b_2\}}{\{b_1\} \in \circ\!\!\circ \ni \{b_3\}} \tag{119}$$

Clearly, none of the labeled graphs (119) allows for nontrivial automorphisms. This may change when multisets are used to generate the labels.

Symmetry factors:

Each unlabeled $t \in \mathcal{T}_n$ has an automorphism group which we define in the obvious way: let ν_0 be the set of open circle vertices, ν_1 the set of dashed vertices, and $\epsilon \subset (\nu_0 \cup \nu_1)_2$ the edge list, subject to the constraints in the definition. An automorphism of t is a permutation of $\nu_0 \cup \nu_1$ that leaves ν_0, ν_1 and the edge list separately invariant. These form a group for which we write $\mathrm{Aut}(t)$.

The labeling process described above precludes nontrivial permutations except when B has repeated elements. For a multiset (117) the m_i copies of b_i can be permuted giving rise to a direct product $\mathrm{Perm}(B) := S_{m_1} \times \ldots \times S_{m_J}$ of symmetric groups acting on B. For a partition $\pi \in \mathcal{S}(B, n)$ let $\nu_0^\pi = \{(o_i, c_i) : i = 1, \ldots, n\}$ be the set of n labeled open circle vertices. Note that each dummy labeled o_i is paired with non-dummy c_i, the index i merely enumerates the list of pairs. Each cell $c_i, i = 1, \ldots, n$ may again be a multiset $\{b_1^{c_{i,1}}, \ldots, b_J^{c_{i,J}}\}$ with multiplicities $c_{i,1}, \ldots, c_{i,J} \in \mathbb{N}_0$, where we set the multiplicity to zero if the element does not occur. A subgroup $\mathrm{Perm}(c_i) = S_{c_{i,1}} \times \ldots \times S_{c_{i,J}} \subset \mathrm{Perm}(B)$ (with factors absent whose multiplicity is zero) will still permute copies of the same elements that c_i may contain. By the very process of forming set partitions the direct product $\mathrm{fix}(\nu_0^B) := \mathrm{Perm}(c_1) \times \ldots \times \mathrm{Perm}(c_n) \subset \mathrm{Perm}(B)$ is still a subgroup, with $S_{c_{1,1}} \times \ldots \times S_{c_{n,1}} \subset S_{m_1}$, etc. In other words, $\mathrm{fix}(\nu_0^B)$ is the subgroup of $\mathrm{Perm}(B)$ that maps individual labels of $T \in \mathcal{T}(B, n)$ into themselves. Writing $|\mathrm{fix}(\nu_0^B)|$ for its order, one has by Lagrange's theorem

$|\mathrm{Perm}(B)|/|\mathrm{fix}(\nu_0^B)| \in \mathbb{N}$.

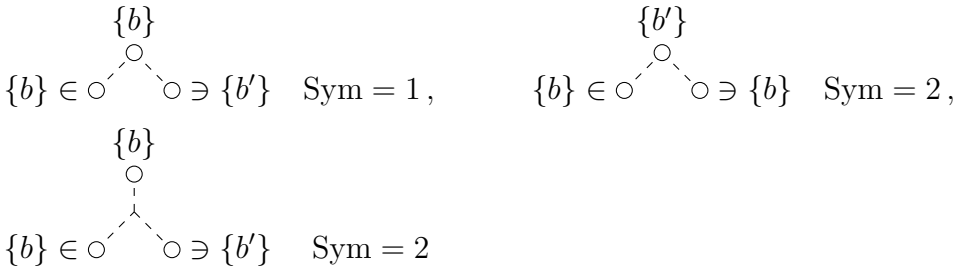
An automorphism of $T \in \mathcal{T}(B,n)$ is defined as in the unlabeled case, except that the unlabeled set ν_0 of $t \in \mathcal{T}_n$ is replaced with the labeled one $\nu_0^\pi = \{(o_i, c_i) : i = 1, \ldots, n\}$, $\pi \in \mathcal{S}(B,n)$. Since the o_i labels are dummy two elements of ν_0^π are regarded as equal iff their cells c_i are equal as multisets. The n labeled vertices can thus be grouped into subsets with the same label. An automorphism of the underlying unlabeled graph t that affects only sets of equally labeled vertices is also an automorphism of T, and all automorphisms of T arise in that way. They form again a group, denoted by $\mathrm{Aut}(T)$, which is a subgroup of $\mathrm{Aut}(t)$. Finally, the *symmetry factor* of a labeled tree graph $T \in \mathcal{T}(B,n)$ is defined by

$$\mathrm{Sym}(T) = |\mathrm{Aut}(T)||\mathrm{fix}(\nu_0^B)|\,. \tag{120}$$

As an illustration of these concepts, reconsider the graphs in (119) but now labeled by the set partitions of $\{b, b, b'\}$. The symmetry factors (120) may differ from 1 and are noted to the right of each graph:

$\{b,b,b'\} \in \circ \quad \mathrm{Sym} = 2$

$\{b\} \in \circ \text{ - - - - } \circ \ni \{b,b'\} \quad \mathrm{Sym} = 1\,, \qquad \{b'\} \in \circ \text{ - - - - } \circ \ni \{b,b\} \quad \mathrm{Sym} = 2\,,$



(121)

We now claim that

$$|\mathrm{Perm}(B)|/\mathrm{Sym}(T) \in \mathbb{N}\,, \tag{122}$$

We present a direct proof on the level of multisets here. In Section 3.4 the result is recovered along different lines. Suppose that $\tilde{p}$ of the elements of ν_0^π of T are equally labeled, and that there is a subgroup A of $\mathrm{Aut}(t)$ that acts transitively on $\{o_1, \ldots, o_p\}$ of t, with $p \leq \tilde{p}$. A may act on vertices other than $\{o_1, \ldots, o_p\}$, once these are labeled only a subgroup A_0 of A may act on the equally labeled $\{(o_j, c_j) : j = 1, \ldots, n\}$, $c_1 = \ldots = c_p$. Note that $p!/|A_0|$ is an

integer. We wish to lift this $A_0 \subset \mathrm{Aut}(t)$ to an automorphism group of the labeled version T of t with the p equally labeled $\{(o_j, c_j) : j = 1, \ldots, p\}$. Focus on one of the elements of the p identical cells c_j with nonzero multiplicity, say $b_1^{c_{j,1}}$, $c_{j,1} = n_1 \geq 1$, $j = 1, \ldots, p$, without loss of generality. Overall these are pn_1 copies of b_1 which arose by distributing the original $m_1 \geq pn_1$ copies from (117) to the cells under consideration and possibly others. Hence there is a subgroup $S_{pn_1} \subset S_{m_1}$ that permutes the copies of b_1 within each cell and mixes the b_1 sectors of different cells. The permutations within each cell are part of $\mathrm{fix}(\nu_0^B)$ and have total order $(n_1!)^p$. The other permutations implement the desired automorphisms of T within S_{pn_1}. The relevant ratio thus is $p!/|A_0| \in \mathbb{N}$ times $(pn_1)!/[p!(n_1!)^p]$. The latter is indeed an integer for all $n_1 \in \mathbb{N}$. Repeating the argument for all elements of the p identical cells with nonzero multiplicities one arrives at $|\mathrm{Perm}(B)|/\mathrm{Sym}(T) \in \mathbb{N}$. This argument does not rely on a group structure of the permutations of elements across cells.

3.3.2 Formulation and illustration of the graph rule

We now return to the previous result (110) and provide a graph rule for the missing ingredient $\mu^\Gamma(v|L)$, where $L \in \mathcal{L}_l$ is a 1LI graph with l edges and v is one of its vertices. Recall the notion of a block decomposition from the end of Section 3.2.1. Each $L \in \mathcal{L}_l$ is either itself 1VI or has a block decomposition $\{L_1, \ldots, L_N\}$, in terms of maximal 1VI subgraphs $L_j = (B_j, E_j)$, $j = 1, \ldots, N$, which must also be 1LI. Each articulation vertex occurs in more than one B_j, while non-articulation vertices occur in precisely one B_j. For a fixed articulation vertex v let $B(v) = \{L_i(v) = (B_i, E_i), i \in I(v)\}$, with $2 \leq |I(v)| \leq N$, be the subset of blocks with $v \in B_i$. Isometric blocks can be permuted, we denote this permutation group by $\mathrm{Perm}(B(v))$ and its order by $|\mathrm{Perm}(B(v))|$. We write $b_i(v)$ for the copy of v in B_i, $i \in I(v)$, and treat the copies $b_i(v)$ as identical, $b_i(v) = b_{i'}(v)$, iff $L_i(V)$ and $L_{i'}(v)$ are isomorphic. Viewed as a vertex in $L_i(v)$ each $b_i(v)$ has a degree (with respect to the full lines) $d(b_i(v)) \geq 2$ such that $\sum_{i \in I(v)} d(b_i(v)) = d(v)$. Non-articulation points can formally be included in this setting by allowing $|I(v)| = 1$.

With this convention the edge sets are redundant and we also write $B(v) = \{b_i(v) : i \in I(v)\}$, on which the same permutation group $\mathrm{Perm}(B(v))$ acts. In general $B(v)$ will

be a multiset for which use the notations (117). Then $\mathrm{Perm}(B(v))$ is a direct product $S_{m_1}\times\ldots\times S_{m_J}$ of symmetric groups. Next we generate the set partitions $\mathcal{S}(B(v),n)$ with $n=1,\ldots,|I(v)|$ cells. Each cell $c_i=\{b_1^{c_{i,1}},\ldots,b_J^{c_{i,J}}\}$ may again be a multiset whose multiplicities obey $\sum_{i=1}^n c_{i,j}=m_j$ and $\sum_{i=1}^n\sum_{j=1}^J c_{i,j}=|I(v)|$. The cells are used to label the open circle vertices of the tree graphs in $\mathcal{T}_n$, $1\le n\le|I(v)|$, as in Section 3.3.1; coinciding labels are allowed and correspond to cells coinciding as multisets. We write $\mathcal{T}(B(v),n)$ for the set of topologically distinct labeled dashed graphs with n open circle vertices labeled by $\mathcal{S}(B(v),n)$. Individual labeled graphs are denoted by $T\in\mathcal{T}(B(v),n)$, with $\mathrm{Sym}(T)$ the symmetry factor.

Theorem 3.3.2 (Graph rules for vertex weights)**.** The weights $\mu^\Gamma(v|L)$ in (110) depend only on the block decomposition $B(v)$ of L at v and can be obtained by the following graph rule:

(a) A weight $\mu(T)$ is assigned to each labeled graph $T\in\mathcal{T}(B(v),n)$, $1\le n\le|I(v)|$, as follows: for an $|o|$-valent (with respect to the dashed lines) open-circle vertex o labeled by the cell $c_i=\{b_1^{c_{i,1}},\ldots,b_J^{c_{i,J}}\}$ write a factor $\omega_{|o|+d(c_i)}(\varphi_v)$, $d(c_i):=\sum_{j=1}^J c_{i,j}d(b_j)$, for each dashed line connecting two open circle vertices a factor $\gamma_2(\varphi_v)$, and for each vertex with $m\ge3$ intersecting dashed lines a factor $\gamma_m(\varphi_v)$ (the dashed lines that intersect at the dashed-vertex do not contribute a factor). The resulting monomial $\mu(T)$ in $\gamma_2,\omega_m,\gamma_m,m\ge3$, has by (113) degree $\sum_{i=1}^n d(c_i)=\sum_{j=1}^J m_j\,d(b_j)=d(v)$.

(b) Multiply $\mu(T)$ by

$$(-)^{s(T)}\frac{|\mathrm{Perm}(B(v))|}{\mathrm{Sym}(T)}\,, \tag{123}$$

where $s(T)$ is the sum of the number of dashed lines and the number of dashed vertices. Further, $|\mathrm{Perm}(B(v))|$ is the order of the permutation group of the blocks at v, and $\mathrm{Sym}(T)$ is the symmetry factor of the labeled dashed graph as defined in Section 3.3.1.

(c) Sum the contributions from (a),(b) over all n and $T\in\mathcal{T}(B(v),n)$ to obtain $\mu^\Gamma(v|L)=\mu^\Gamma(v|B)$ as

$$\mu^\Gamma(v|B)=\sum_{n=1}^{|I(v)|}\sum_{T\in\mathcal{T}(B(v),n)}(-)^{s(T)}\frac{|\mathrm{Perm}(B(v))|}{\mathrm{Sym}(T)}\mu(T)\,. \tag{124}$$

This is normalized such that $\mu^\Gamma(v|L)=\omega_{d(v)}(\varphi_v)$ for a non-articulation vertex ($|I(v)|=1$) of degree $d(v)$.

Illustration of the graph rule:

(i) The simplest case is the "pair of glasses" graph in (101). It has two isomorphic blocks  , joined at the articulation point. Hence $|\mathrm{Perm}(B(v))| = 2$. The vertex set $B(v)$ contains two copies of the same element, $\{b, b\}$, say, with $d(b) = 2$. The set partitions of $B(v)$ are $\{\{b, b\}\}$ and $\{\{b\}, \{b\}\}$. Thus the labeled dashed graphs $T \in \mathcal{T}(B(v), 1), \mathcal{T}(B(v), 2)$, are

$$\{b, b\} \in \circ, \quad \{b\} \in \circ \text{- - -} \circ \ni \{b\}. \tag{125}$$

They have each $\mathrm{Sym}(T) = 2$, and contribute $\omega_4(\varphi)$, $-\gamma_2(\varphi)\omega_3(\varphi)^2$, respectively, in the sum (124). This reproduces the weight in (101).

(ii) As a more complicated exemplification consider (107). At v' three block are joined: two copies of  , and  . Hence $|\mathrm{Perm}(B(v'))| = 2$. The vertex set $B(v') = \{b, b, b'\}$ with $d(b) = 2$, $d(b') = 3$, gives rise to the labeled tree graphs presented in (121). The sum (124) evaluates to

$$\begin{aligned}\mu(v'|L) = {} & \frac{2}{2}\omega_7(\varphi_{v'}) - \frac{2}{1}\gamma_2(\varphi_{v'})\omega_3(\varphi_{v'})\omega_6(\varphi_{v'}) - \frac{2}{2}\gamma_2(\varphi_{v'})\omega_4(\varphi_{v'})\omega_5(\varphi_{v'}) \\ & + \frac{2}{2}\gamma_2^2(\varphi_{v'})\omega_3^2(\varphi_{v'})\omega_5(\varphi_{v'}) + \frac{2}{1}\gamma_2^2(\varphi_{v'})\omega_3(\varphi_{v'})\omega_4^2(\varphi_{v'}) + \frac{2}{2}\gamma_3(\varphi_{v'})\omega_3^2(\varphi_{v'})\omega_4(\varphi_{v'}),\end{aligned} \tag{126}$$

in agreement with (107). At v two distinct blocks are joined,  and  . Hence $|\mathrm{Perm}(B(v))| = 1$. The vertex set is $B(v) = \{b, b'\}$, with $d(b) = 2$, $d(b') = 3$. The labeled tree graphs are as in (125) but with distinct elements b, b'. Both have symmetry factor 1 and the sum (124) gives $\mu(v|L) = \omega_5(\varphi_v) - \gamma_2(\varphi_v)\omega_3(\varphi_v)\omega_4(\varphi_v)$, again in agreement with (107).

3.3.3 Proof of the graph rule

We first bring into focus what needs to be shown. By Lemma 3.3.1 each weight $\mu^\Gamma(v|L)$ lies in the direct sum of $\mu(\mathcal{T}_n^D), n = 1 \ldots, n_{\max}$, $n_{\max} \leq d(v) - 3$, for some integer multiset D_n. It is convenient to introduce a projection operation

$$\mathrm{pr} : \mathcal{T}(B(v), n) \longrightarrow \mathcal{T}(D(v), n)\,, \quad T \mapsto \mathrm{pr}(T)\,, \tag{127}$$

where $D(v) = d(B(v))$, as a multiset. Further, each cell c_i labeling $T \in \mathcal{T}(B(v), n)$ is replaced by its integer degree sum $d(c_i)$. The result is an element of $\mathcal{T}_n^D$, where the integers D_n are

$d(\pi) := \{d(c_1), \ldots, d(c_n)\}$ (viewed as a multiset), if $\pi = \{c_1, \ldots, c_n\}$ is the partition labeling T. Note that each D_n is drawn from the n-element partitions of $D(v) = \{d(b_i) : i \in I(v)\}$, with each integer in D_n equal to the sum of the integers in the cell. Since distinct b_i's can have the same degree and many degree sums $d(c_i)$ can be equal as well, the projected label set $\mathcal{S}(D(v), n)$ will in general be of much smaller cardinality than $\mathcal{S}(B(v), n)$. We write $\mathcal{T}(D(v), n)$ for the set of topologically inequivalent labeled dashed graphs with n open circle vertices labeled by some $D_n \in \mathcal{S}(D(v), n)$.

Clearly, $\mu(T) = \mu(\tau)$, for $\tau = \mathrm{pr}T$, if $\mu(\tau)$ is formed according to (114). The graph rule is therefore compatible with Lemma 3.3.1 and the projection (127). What remains to be shown is: $n_{\max} = |I(v)|$, and

$$\text{coefficient of } \mu(T) = (-)^{s(T)} \frac{|\mathrm{Perm}(B(v))|}{\mathrm{Sym}(T)}\,, \quad T \in \mathcal{T}(B(v), n)\,,\ n = 2, \ldots n_{\max}\,. \tag{128}$$

The case $n = 1$ is accounted for by (109) and can be omitted. Indeed, for $n = 1$ the only $T \in \mathcal{T}(B(v), 1)$ graph is an open circle labeled by $c_1 = B(v)$, the groups $\mathrm{Perm}(B(v))$ and $\mathrm{fix}(\nu_0^B)$ coincide and the coefficient of $\mu(T) = \omega_{d(v)}$ is 1, in agreement with (109). By Lemma 3.2.2 we can also match the situation where only the $\omega_{d(v)}$ term in (127) is present to graphs L without articulation points, in agreement with the graph rule. The key step is:

Lemma 3.3.3. *For 1LI graphs with one articulation point (128) and hence the graph rule (a),(b),(c) is compatible with the recursion (98).*

Proof. We proceed by induction in l by assuming that (a), (b), (c) of the graph rule produce the correct vertex expressions for orders $1, \ldots, l-1$. Let $L \in \mathcal{L}_l$ be a 1LI graph with a single articulation vertex v, and $L_1(v), \ldots, L_I(v)$ is its block decomposition. The $L_i(v)$ are viewed as 1-rooted graphs, with roots b_i regarded as identical iff the $L_i(v)$ are isomorphic as 1VI graphs. With this convention $B(v)$ is a multiset of the form (117) which codes the structure of L at v. In the recursion (98) the contribution coming from L is reassembled from its block decomposition by gluing together various blocks arising from the graph expansion of the $W^{(k)}_{l-m}$, $\Gamma^{(1)}_{m_1}, \ldots, \Gamma^{(1)}_{m_k}$ pieces. The weights associated with non-articulation vertices are known from Lemma 3.2.2 so we can focus on v.

At v the structure of the 1LI graph L^W induced by $W^{(k)}_{l-m}$ is irrelevant (as in the proofs

of Lemmas 3.3.1 and 3.3.4) and only the shifted weight ω_{d_0+k} enters, where $d_0 = d(v_0)$ is the valency (wrt the full lines) of v's copy v_0 in the 1LI graph associated with W_{l-m}. The shift counts the number of h-derivatives acting on $\omega_{d_0}(h)|_{h=H_v}$; since L has by assumption only one articulation point all k derivatives in $W^{(k)}_{l-m}$ must act on the same vertex weight, viz $\omega_{d_0}(h)$. In particular v_0 should be viewed a rooted vertex with multiplicity k. Attached to v_0 will be k 1LI graphs $L^\Gamma_j \in \mathcal{L}^{1\bullet}_{m_j}$ that arise from the graph expansion of $\Gamma^{(1)}_{m_j}$, respectively, and that are rooted at some v_j. Each of the L^Γ_j may decompose into several blocks at v_j, in the above convention we may write $B(v_j)$ for the set of blocks stemming from $L^\Gamma_j \in \mathcal{L}^{1\bullet}_{m_j}$. Similarly, L^W may decompose into several blocks at v_0 and we write $B(v_0)$ for their vertex set. Then $B(v)$ is the union of the $B(v_j)$, $j = 0, 1, \ldots, k$, as k runs through all possible values in (98). For fixed k the weight associated with v can be written in terms of its copies in $B(v_j)$ as

$$\omega_{d(v_0)+k} \prod_{j=1}^{k} \partial_\varphi \mu^\Gamma(v_j|B(v_j)) \,, \quad k = 1, \ldots, [m/2] \,, \tag{129}$$

where by induction hypothesis each $\mu^\Gamma(v_j|B(v_j))$ is given by (124). In particular, each $\mu^\Gamma(v_j|B(v_j))$ expands into contributions associated with dashed graphs in $\mathcal{T}(B(v_j), n_j)$, $n_j = 1, \ldots, |I(v_j)|$, labeled by the set partitions of $B(v_j)$ with n_j cells, $j = 1, \ldots, k$. The minimal number of cells is k, the maximal number of cells is $\sum_{j=1}^k |I(v_j)| = |I(v)| - 1$. The blocks in $B(v_0)$ are not subject to the Γ graph rule but to the W graph rule and thus only give rise to the $\omega_{d(v_0)+k}$ factor in (129). In terms of the integer labeled dashed graphs $d(v_0)$ labels a k-valent open circle vertex $o \in \nu_0$ and conversely every k-valent open circle vertex in an integer labeled dashed graph can be associated with a $W^{(k)}_{l-m}$ induced piece. Each of the k-subtrees joined to it has a dashed edge generated by ∂_φ without open circle vertex, while all of its n_j open circle vertices are labeled by the set partitions in $\mathcal{S}(n_j, B(v_j))$, $j = 1, \ldots, k$. The result is a dashed graph T' with $n = 1 + \sum_{j=1}^k n_j \in \{k+1, \ldots, |I(v)|\}$ open circle vertices, all but one of which are labeled by set partitions drawn from those of the individual $B(v_j)$'s. In the setting of (128) this fixes $n_{\max} = |I(v)|$. Subject to the degree constraint $d(c_0) = d(v_0)$ the so far only integer labeled vertex v_0 can also be labeled by some vertex set c_0.

We are free to postulate that T' ought to be relabeled – while preserving the weight – by the much larger set of set partitions of $B(v)$, viewed as the union of $B(v_j)$, $j = 0, 1, \ldots, k$,

to produce a graph in $T \in \mathcal{T}(B(v), n)$, $n = k+1, \ldots, |I(v)|$. For later reference we mark the transition from T' to T with $\mu(T') = \mu(T)$ by $(*)$. Summing the contributions (129) over all $k = 1, \ldots, [m/2]$, $m = 2, \ldots, l-2$, we know that the result must be of the form (124) but with a yet undetermined coefficient of $\mu(T)$. As noted after (127) the weight only depends on the projection $\mathrm{pr}(T)$ of the graph, but we are free to stipulate that the integers occurring are the degree sums of the cell partitions of $B(v)$, i.e. $d_i = d(c_i)$. Then part (a) of the graph rule holds by construction and only the assertion about coefficient (128) needs to be shown.

By the induction hypothesis each the $\Gamma^{(1)}_{m_j}$ induced pieces comes with a $1/\mathrm{Sym}(L^\Gamma_j)$ factor where $L^\Gamma_j \in \mathcal{L}^{1\bullet}_{m_j}$ is a 1-rooted 1LI graph. Similarly, by the W graph rule the $W^{(k)}_{l-m}$ induced piece carries a $1/\mathrm{Sym}(L^W)$ factor, where L^W is also a 1-rooted 1LI graph but with the root attributed multiplicity k, as seen above. Since we focus on 1LI graphs that combine to L (and L has only one articulation point) all $L^W, L^\Gamma_1, \ldots, L^\Gamma_k$, have a clover-like block decomposition with the blocks joined at a central vertex $v_0, v_1, \ldots, v_k$, respectively. Each block is treated as 1-rooted and arranged in some lexicographic order that they can be identified with the blocks $L_1, \ldots, L_I$ of L at v. The prefactor of a term on the right hand side of (98) contributing to L via the $k+1$ 1LI subgraphs is thus

$$\frac{1}{\mathrm{Sym}(L^W)} \prod_{j=1}^{k} \frac{1}{\mathrm{Sym}(L^\Gamma_j)} = \prod_{j=0}^{k} \frac{1}{|\mathrm{Perm}(B(v_j))|} \prod_{i=1}^{I} \frac{1}{\mathrm{Sym}(L_i)} \,. \tag{130}$$

This collects all the pre-factors arising from (85), (110) and we proceed to the normalized weight for the articulation vertex v obtained from (98).

Each $\partial_\varphi \mu(v_j | B(v_j))$ in (129) expands into tree graphs $\{T_j\}$ which we regard as 1-rooted, $\{T_j\} \subset \mathcal{T}^{1\bullet}_{n_j}$, and the root as the endpoint of a dashed edge without open circle. The normalized weight at v_j carries the coefficient

$$(-)^{|\nu_1(T_j)|+|\epsilon(T_j)|} \frac{|\mathrm{Perm}(B(v_j))|}{\mathrm{Sym}(T_j)}, \quad \{T_j\} \subset \mathcal{T}^{1\bullet}_{n_j}, \tag{131}$$

with the symmetry factor defined in (120). For $j = 1, \ldots, k$ the $|\mathrm{Perm}(B(v_j))|$ cancels against that in (130). Suppose now for fixed $j \in \{1, \ldots, k\}$ there are k_j isomorphic subtrees T_j (not separately named) attached to the $W^{(k)}_{l-m}$ vertex, with $\sum_j k_j = k$. Then accounting for the $1/k!$ in (98) and omitting the $\prod_{i=1}^{I} 1/\mathrm{Sym}(L_i)$ from (130) we obtain the full prefactor of the

choice of $W^{(k)}_{l-m}$ vertex

$$\frac{1}{|\mathrm{Perm}(B(v_0))|}\prod_{j=1}^{k}\left(\frac{(-)^{k_j(|\nu_1(T_j)|+|\epsilon(T_j)|)}}{k_j!\,\mathrm{Sym}(T_j)^{k_j}}\right). \tag{132}$$

Let $T\in\mathcal{T}(B(v),n)$, $n=1+\sum_{j=1}^{k}n_j$, (in the notation introduced after (129)) be the graph reassembled from the rooted subtrees T_j at the vertex o with weight $\omega_{k+d(v_0)}$. The total weight is $\omega_{k+d(v_0)}$ times the products of the weights of the subtrees, and is of the form $\mu(T)$ in part (a) of the graph rule. The overall sign is $(-)^{|\nu_1(T)|+|\epsilon(T)|}=(-)^{s(T)}$. A straightforward application of the orbit stabilizer theorem shows that the modulus of (132) equals

$$\frac{1}{|\mathrm{fix}(\nu_0^B)||\mathrm{Aut}(T^1)|}, \tag{133}$$

where T^1 is T seen as rooted at the open circle vertex o. Further, we used that $\mathrm{fix}(\nu_0^B)$ is a direct product over cells and treated the $\mathrm{Perm}(B(v_0))$ from (132) as the factor in $\mathrm{fix}(\nu_0^B)$ associated with the v_0 cell. There may be several identical choices for the k-valent open circle vertex o introduced after (129) and this is just $\mathrm{orb}(o)$, the orbit of o under $\mathrm{Aut}(T)$. Taking into account (120) and the $(l-m)/l$ from (98) the net coefficient is

$$\frac{(-)^{s(T)}}{\mathrm{Sym}(T)}|\mathrm{orb}(o)|\times\frac{l-m}{l}. \tag{134}$$

Each of these k-valent open circle vertices o is labeled by a cell containing the vertices $b_i(v)\in B_i$ of some subset of blocks $L_i=(B_i,E_i)$, $i\in I_o$, and we usually omit the edge set E_i. Restoring some of the information we may attribute to o the total number $l(o)=\sum_{i\in I_o}|E_i|$ of solid lines in the blocks labeling it. Then $\sum_{o\in\nu_0^B}l(o)=|E|$ is the total number of edges in the original graph with one articulation vertex.

We now apply this to the clover like 1LI graph L^W with $l-m$ edges. After the relabeling $T'\mapsto T$ described at $(*)$ the relevant vertex set is ν_0^B, $B=B(v)$, with the blocks attributed to o such that $l(o)=l-m$. The point of the re-interpretation is each orbit in $\nu_0^B/\mathrm{Aut}(T)$ corresponds to a distinct choice of the $W^{(k)}_{l-m}$ piece, and the contribution (134) of T to $\mu(v|L)$ involves

$$\sum_{[o]\in\nu_0^B/\mathrm{Aut}(T)}|\mathrm{orb}(o)|l(o)=\sum_{o\in\nu_0^B}l(o)=l\,. \tag{135}$$

Summing (134) using (135) the coefficient of $\mu(T)$ is $(-)^{s(T)}/\mathrm{Sym}(T)$. Finally, restoring the

$$\prod_{i=1}^{I} \frac{1}{\mathrm{Sym}(L_i)} = \frac{|\mathrm{Perm}(B)|}{\mathrm{Sym}(L)}\,, \tag{136}$$

from (130) and the $\mu(T)$ itself the normalized contribution of the articulation vertex v is

$$(-)^{s(T)} \frac{|\mathrm{Perm}(B(v))|}{\mathrm{Sym}(T)} \mu(T), \tag{137}$$

as claimed by the graph rule. □

Next we show a 'locality' result which allows one to reduce the case with multiple articulation points to that with just one.

Lemma 3.3.4. *(Locality) The recursion (98) implies that the weights $\mu^\Gamma(v|L)$, $L \in \mathcal{L}_l$, depend only on the block decomposition $B(v) = \{L_i(v) = (B_i, E_i) : i \in I(v)\}$ of L at v, symbolically*

$$\mu^\Gamma(v|L) = \mu^\Gamma(v|B)\,, \tag{138}$$

where on the right hand side $\mu^\Gamma(v|\,\cdot\,)$ is regarded as a map from $B(v)$ to the smooth functions in φ_v.

Proof. By (109) we know the structure of $\mu^\Gamma(v|L)$ but the coefficients could in principle depend on all aspects of the graph L to which v belongs. To exclude this, we retain the notation from the preceeding Lemma and trace the changes that occur if the original L has more than one articulation point. We single out one articulation point v write v_0 for its copy in the 1LI graph L^W. In the paragraph leading to (129) then any number $r = 1, \ldots, k$ of h derivatives can act on the $\omega_{d_0}(h)|_{h=H_v}$, in which case v_0 should be viewed as a root with multiplicity r. Attached to v_0 will be r 1LI graphs selected from the $L_j^\Gamma \in \mathcal{L}^{1\bullet}_{m_j}$, $j = 1, \ldots, k$. Without loss of generality we may take L_j^Γ, $j = 1, \ldots, r$, as the 1LI graphs attached to v_0. We write again $B(v_j)$ for the vertex set blocks stemming from L_j^Γ and $B(v_0)$ for the vertex set of the L^W blocks at v_0. Then $B(v)$ is the union of $B(v_0)$ and $B(v_j), j = 1, \ldots r$, as $1 \le r \le k \le [m/2]$ runs through all possible values allowed by (98). For any fixed r the

weight associated with v is

$$\omega_{d(v_0)+r} \prod_{j=1}^{r} \partial_\varphi \mu^\Gamma(v_j|B(v_j))\,. \tag{139}$$

With the replacement of k by r the reasoning after (129) carries over and establishes in particular $n_{\max} = |I(v)|$. The relabeling $(*)$ from T' to T proceeds as before, with k replaced by r. Summing the contributions (139) over all allowed $1 \le r \le k \le [m/2]$ must result in a weight of the form (127) with $n_{\max} = |I(v)|$. The $\mu(T)$ obtained is solely determined by block structure of L at v and adheres to the graph rule. The way the coefficient of $\mu(T)$ is computed by the recursion (98), however, initially refers to pieces of information not localized at v.

In pinning down the coefficient of $\mu(T)$ the key difference to the previous Lemma is that the relevant 1-rooted 1LI graphs L^W (multiplicity r) and $L_1^\Gamma, \dots, L_r^\Gamma$ (all multiplicity 1) no longer have to have a clover like structure. That is, in addition to articulation vertex v_0 and $v_1, \dots, v_r$ in focus these graphs can have other articulation vertices. This complicates the reduction of the symmetry factors $\mathrm{Sym}(L^W)$, $\mathrm{Sym}(L_1^\Gamma), \dots, \mathrm{Sym}(L_r^\Gamma)$, to those of the constituent blocks. However (130) remains valid if the L_i on the right hand side are interpreted as the not necessarily 1VI subgraphs that arise by disassembling the L^W, $L_1^\Gamma, \dots, L_r^\Gamma$, at v_0, $v_1, \dots, v_r$, respectively. With this reinterpretation the structure of the L^W, $L_1^\Gamma, \dots, L_r^\Gamma$, remains clover-like at the vertex in focus. The line of reasoning from (131) to (134) carries over with k replaced by r and so does the remainder of Lemma 3.3.3. In summary, the pieces of information (130), (134), (136) referring to the global structure of the reassembled graph L cancel out in the final result for the coefficient of $\mu(T)$, which has the form demanded in (128). □

Combined, Lemma 3.3.3 and Lemma 3.3.4 imply Theorem 3.3.2.

3.4 Reduction to integer labeled trees

Our formula (124) for the $\mu^\Gamma(v|L)$ weight at v renders the 'locality' of the data $B(v)$ determining it manifest. The labeling of the tree graphs $\mathcal{T}(B(v), n), n = 1, \dots, |I(v)|$, by the

set partitions of $B(v)$ is a convenient way to account for the coefficients with which a certain monomial in $\gamma_2, \gamma_m, \omega_m$, $m \geq 3$, occurs. Comparing with (127), (128) one may suspect that the labeling by vertex set partitions $\{c_1, \ldots, c_n\} \in \mathcal{S}(B(v), n)$ somewhat overspecifies the necessary data. Indeed, upon identifying the integers d_i in (114), (115) with $d_i = d(c_i)$, the sum of the vertex degrees in cell c_i, one expects $\mu^\Gamma(v|B)$ to depend only on these integers, not on the details of the labeling cells c_i themselves. This turns out to be the case because subsums in (124) with fixed $\mu(T)$ can be performed and manifestly depend only the unlabeled tree and the $d(c_i)$. To avoid complications due to accidental degeneracies we sum over a subset of graphs whose defining criterion is sufficient but not necessary for the constancy of $\mu(T)$.

We return to the projection (127) and note that the weight $\mu(T)$ depends only on $\mathrm{pr}(T) = \tau$. Indeed, with $\mu(\tau)$ formed according to (114), one has $\mu(T) = \mu(\tau) = m(t) \prod_{i=1}^n \omega_{r_i}$, where $m(t)$ collects the γ_m, $m \geq 2$, factors that depend only on the unlabeled graph. The integers $r_i = \mathrm{ddeg}(o_i, d(c_i))$ lie in the range of the ddeg function (112) and depend only on the integer labeled vertex set $\mathrm{pr}\nu_0^\pi = \nu_0(\tau)$, $\tau \in \mathcal{T}_n^{d(\pi)}$. Here $d(\pi)$ can be any element of the projected label set $\mathcal{S}(D(v), n)$ as defined after (127). It is convenient to introduce for given $t \in \mathcal{T}_n$, $D_n \in \mathcal{S}(D(v), n)$, the range of ddeg acting on the vertex set $\nu_0(\tau)$ of some $\tau \in \mathcal{T}_n^D$

$$\rho(t, D_n) = \{\mathrm{ddeg}\nu_0(\tau) : \tau \in \mathcal{T}_n^D\}\,. \tag{140}$$

For $n \geq 2$ elements ρ_n of $\rho(t, D_n)$ are of the form $\rho_n = \{3 \leq r_i \in \mathbb{N} : i = 1, \ldots, n\}$ and the weight $\mu(\tau) = \mu(t, \rho_n)$ only depends on t and $\rho_n \in \rho(t, D_n)$. We seek to identify labeled graphs $T \in \mathcal{T}(B(v), n)$ with fixed $\mu(T)$; by the previous considerations this requires to hold for given t, D_n the $\rho_n \in \rho(t, D_n)$ fixed. We thus write $\mathcal{T}(t, B(v), n)$ for the set of topologically inequivalent dashed graphs that arise by labeling $t \in \mathcal{T}_n$ with $\mathcal{S}(B(v), n)$. Defining

$$\mathcal{T}^B(t, D_n, \rho_n) := \{T \in \mathcal{T}(t, B(v), n) : \mathrm{pr}T = \tau \in \mathcal{T}_n^D\,,\ \mathrm{ddeg}(\mathrm{pr}\nu_0^\pi) = \rho_n\}\,, \tag{141}$$

all its elements have the same weight $\mu(t, \rho_n)$. Further, the full set of labeled dashed graphs can be partitioned according to

$$\mathcal{T}(t, B(v), n) = \bigcup_{D_n \in \mathcal{S}(D(v), n)} \bigcup_{\rho_n \in \rho(t, D_n)} \mathcal{T}^B(t, D_n, \rho_n)\,. \tag{142}$$

The image under pr of the union of (142) over all $t \in \mathcal{T}_n$ is partitioned analogously,

$$\mathcal{T}(D(v), n) = \bigcup_{D_n \in \mathcal{S}(D(v),n)} \bigcup_{t \in \mathcal{T}_n} \bigcup_{\rho_n \in \rho(t, D_n)} \mathcal{T}_n^D(\rho_n)\,, \tag{143}$$

with $\mathcal{T}_n^D(\rho_n) := \{\tau \in \mathcal{T}_n^D : \mathrm{ddeg}\nu_0(\tau) = \rho_n\}$. In the graph rule formula (124) the decomposition (142) allows one to 'pull in' the sub-sub over $\mathcal{T}^B(t, D_n, \rho_n)$. The evaluation of this subsum is the main result of this section:

Theorem 3.4.1. In the graph rule (124) the sum over graphs $T \in \mathcal{T}(B(v), n)$ labeled by partitions of the vertex set $B(v)$ can be replaced with a sum over *integer* labeled trees. Specifically, $\mu^\Gamma(v|B) = \mu^\Gamma(v|D)$, with $D(v) = d(B(v))$ and

$$\begin{aligned} \mu^\Gamma(v|D) &= \sum_{n=1}^{|I(v)|} \sum_{D_n \in \mathcal{S}(D(v),n)} \sum_{t \in \mathcal{T}_n} (-)^{s(t)} \sum_{\rho_n \in \rho(t, D_n)} c(t, D_n, \rho_n) \mu(t, \rho_n)\,, \\ c(t, D_n, \rho_n) &= \sum_{T \in \mathcal{T}^B(t, D_n, \rho_n)} \frac{\mathrm{Perm}(B(v))}{\mathrm{Sym}(T)} = \frac{|\nu_0(D_n, \rho_n)|}{|\mathrm{Aut}(t)|} P(D(v), D_n)\,. \end{aligned} \tag{144}$$

Here $P(D(v), D_n)$ is the number of partitions of $|I(v)|$ distinct labels $\{b_1, \ldots, b_{|I(v)|}\}$ into n cells such that the sum of the $d(b_j)$ in the i-th cell cell equals the given d_i, and $|\nu_0(D_n, \rho_n)|$ is the cardinality of $\{\nu_0^\pi : \mathrm{ddeg}(\mathrm{pr}\nu_0^\pi) = \rho_n,\ \pi \in \mathcal{S}(B(v), D_n)\}$. For the latter one has explicitly

$$|\nu_0(D_n, \rho_n)| = \Big(\prod_{i=1}^k n_i!\Big) \prod_{j=1}^n \frac{s_j!}{s_{j,1}! \ldots s_{j,k}!}, \tag{145}$$

where $n_1, \ldots, n_k$, $\sum_{i=1}^k n_i = n$, are the numbers of equally valent open circle vertices in t, and $s_{j,i}$ is the number of equally valent open circle vertices of type i labeled by d_j, where $D_n = \{d_1^{s_1}, \ldots, d_n^{s_n}\}$.

The notational complexity notwithstanding, the formula (144) is in fact a simplification compared to (124) as a much smaller set of labeled trees need to be considered. Before turning to the proof we illustrate the statement in the examples from Sections 2.2 and 2.3. The possible $D(v)$'s for the examples considered in Sections 2.2, 2.3 are $D(v) = \{2, 2\}$, $\{2, 3\}$, $\{2, 2, 3\}$. Theorem 3.4.1 produces the correct weights for each $D(v)$ with cardinality 2 by inspection. As a simple illustration of Theorem 3.4.1, we detail the constituents for $D(v) = \{2, 2, 3\}$.

$n=1$: $D_1=\{7\}$, $P(D(v),D_1)=1$.

$$7\ \circ \qquad \rho_1=\{7\} \quad \tfrac{|\nu_0(D_1,\rho_1)|}{|\mathrm{Aut}(t)|}=1 \tag{146}$$

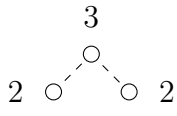
$n=2$: $D_2=\{2,5\}$, $P(D(v),D_2)=2$.

$$2\ \circ\text{- - -}\circ\ 5 \qquad \rho_2=\{3,6\} \quad \tfrac{|\nu_0(D_2,\rho_2)|}{|\mathrm{Aut}(t)|}=\tfrac{2!}{2!}=1 \tag{147}$$

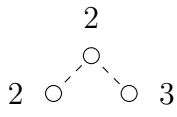
$D_2=\{3,4\}$, $P(D(v),D_2)=1$.

$$3\ \circ\text{- - -}\circ\ 4 \qquad \rho_2=\{4,5\} \quad \tfrac{|\nu_0(D_2,\rho_2)|}{|\mathrm{Aut}(t)|}=\tfrac{2!}{2!}=1 \tag{148}$$

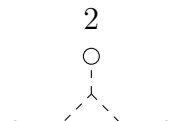
$n=3$: $D_3=\{2,2,3\}$, $P(D(v),D_3)=1$.



$\rho_3=\{3,3,5\}$ $\quad \tfrac{|\nu_0(D_3,\rho_3)|}{|\mathrm{Aut}(t)|}=\tfrac{2!}{2!}=1$



$\rho_3=\{3,4,4\}$ $\quad \tfrac{|\nu_0(D_3,\rho_3)|}{|\mathrm{Aut}(t)|}=\tfrac{2!^2}{2!}=2$



$\rho_3=\{3,3,4\}$ $\quad \tfrac{|\nu_0(D_3,\rho_3)|}{|\mathrm{Aut}(t)|}=\tfrac{3!}{3!}=1$ (149)

This yields $\omega_7-2\gamma_2\omega_3\omega_6-\gamma_2\omega_4\omega_5+\gamma_2^2\omega_3^2\omega_5+2\gamma_2^2\omega_3\omega_4^2+\gamma_3\omega_3^2\omega_4$, in agreement with the result in (104) and (107).

In preparation of the proof of Theorem 3.4.1 we note that $\mathrm{pr}T=\tau\in\mathcal{T}_n^D$ implies that the set partitions π labeling $T\in\mathcal{T}(B(v),n)$ are constrained to lie in $\mathcal{S}(B(v),D_n):=\{\pi\in\mathcal{S}(B(v),n)\,|\,d(\pi)=D_n\}$. These are viewed as (constrained) multiset partitions in the sense explicated after (117). For the subsequent proofs a realization of the multisets as sets of distinct elements $B=\{b_1,\ldots,b_I\}$ modulo an equivalence relation is convenient (to avoid further complicating the notation we write $B(v)$ for the multiset and B for $\{b_1,\ldots,b_I\}$ equipped with an equivalence relation). For the moment we merely stipulate the existence of an equivalence relation "$\sim$" on B compatible with the degree assignments, i.e. $b_i\sim b_j$

implies $d(b_i) = d(b_j)$ but not necessarily vice versa. We denote by $\mathrm{Perm}(B)$ the subgroup of S_I that permutes equivalent b_i's. In this setting the counterpart of the constrained multiset partitions $\mathcal{S}(B(v), D_n)$ is $\bar{\mathcal{S}}(B, D_n) = \mathcal{S}(B, D_n)/\mathrm{Perm}(B)$, while $\mathcal{S}(\{b_1, \ldots, b_I\}, D_n)$ does not depend on the equivalence relation and neither does its cardinality $P(D(v), D_n)$. The counterpart of $\mathcal{T}^B(t, D_n, \rho_n)$ is $\overline{\mathcal{T}}^B(t, D_n, \rho_n)$, the set of labeled graphs obtained by labeling $t \in \mathcal{T}_n$ with $C \in \bar{\mathcal{S}}(B, D_n)$ such that $\mathrm{ddeg}(\mathrm{pr}\nu_0^C) = \rho_n$. The latter condition defines the vertex set $\nu_0(D_n, \rho_n)$. In this setting we later show:

Proposition 3.4.1. Let $B = \{b_1, \ldots, b_I\}$ be a set of distinct vertices equipped with an equivalence relation "$\sim$" that is compatible with the degrees, *i.e.* $b_i \sim b_j$ only if $d(b_i) = d(b_j)$. Define $\mathcal{T}(D_n, \rho_n)$, $\nu_0(D_n, \rho_n)$, and $P(D(v), D_n)$, as above. Then:

$$\sum_{T \in \overline{\mathcal{T}}^B(t, D_n, \rho_n)} \frac{|\mathrm{Perm}(B)|}{\mathrm{Sym}(T)} = \frac{P(D(v), D_n)|\nu_0(D_n, \rho_n)|}{|\mathrm{Aut}(t)|}, \tag{150}$$

is independent of the equivalence relation on B.

Theorem 3.4.1 is an easy consequence of Proposition 3.4.1: Using (142) in (124) (and the fact that $s(T) = s(t)$ is manifestly labeling independent) one finds (144) with the $c(t, D_n, \rho_n)$ given by the sum over $T \in \mathcal{T}^B(t, D_n, \rho_n)$. Since $\sum_{T \in \mathcal{T}^B(t, D_n, \rho_n)} |\mathrm{Perm}(B(v))|/\mathrm{Sym}(T) = \sum_{T \in \overline{\mathcal{T}}^B(t, D_n, \rho_n)} |\mathrm{Perm}(B)|/\mathrm{Sym}(T)$, the second line of (144) follows from (150). The formula (145) is straightforward combinatorics.

Keeping the integer labels from D_n fixed, the dummy labels of the equally valent open circle vertices may be permuted while preserving ρ_n. This contributes the factor $\prod_{i=1}^k n_i!$. The remaining factor follows from the number of ways the s_j labels with degree d_j can be distributed amongst the $n_1, \ldots, n_k$ equally labeled vertices. Application of the multinomial theorem gives the contribution $\prod_{j=1}^n s_j!/(s_{j,1}! \ldots s_{j,k}!)$, and hence the result (145).

It remains to establish Proposition 3.4.1. Its proof is broken up into several lemmas, some of them more general than needed.

Lemma 3.4.2. *Let B, "$\sim$", and* $\mathrm{Perm}(B)$ *be as in Prop. 3.4.1 and* $\mathrm{Sym}(T)$ *as in (120). Then the ratios* $|\mathrm{Perm}(B)|/\mathrm{Sym}(T)$ *are integers, and so are the $d_{i_3, \ldots i_{m-1}}$ in (109).*

Proof. The second part follows trivially from the first. The $\mu(T)$ in (124) refer to a mixed basis of $\gamma_2, \omega_m, \gamma_m$, $m \geq 3$. By Appendix B the transition from $\omega_m(\varphi)$ to $\gamma_n(\varphi)$'s involves

integer coefficients only. It follows that the coefficients in (109) are also integers, $d_{i_3,\ldots i_{m-1}} \in \mathbb{Z}$.

For the first part, recall that labels are generated from the set partitions $\mathcal{S}(B,n)$ of B into n cells. Any resulting partition $\pi = \{c_1,\ldots,c_n\}$ carries an induced equivalence relation defined by $c_i \sim c_{i'}$ iff there is a (possibly non-unique) $\sigma \in \mathrm{Perm}(B)$ such that $\sigma(c_i) = c_{i'}$. This implies that the subset

$$\mathrm{stab}(\pi) = \{\sigma \in \mathrm{Perm}(B) : \forall i\, \exists i' \in \{1,\ldots,n\} \text{ s.t. } \sigma(c_i) = c_{i'}\}, \tag{151}$$

is a subgroup of $\mathrm{Perm}(B)$. The case $i = i'$ in (151) is allowed and gives rise to a subgroup $\mathrm{fix}(\pi) \subset \mathrm{stab}(\pi)$, which in the multiset formulation corresponds to $\mathrm{fix}(\nu_0^B)$. In fact,

$$\mathrm{fix}(\pi) = \{\sigma \in \mathrm{stab}(\pi) : \forall i\, \sigma(C_i) = C_i\} \quad \text{is a normal subgroup of } \mathrm{stab}(\pi). \tag{152}$$

Recall, $H \subset G$ is a normal subgroup if $\forall g \in G$, $g^{-1}Hg = H$. Here, let $\sigma \in \Phi(\pi)$, $\sigma_1 \in \Phi_1(\pi)$. For each i, $\sigma(c_i) = c_{i'}$, $\sigma^{-1}(c_{i'}) = c_i$ with $c_i \sim c_{i'}$. Note that σ may not be unique but any given σ has a unique inverse. Hence, $\sigma_1\sigma(c_i) = c_{i'}$ and $\sigma^{-1}\sigma_1\sigma(c_i) = c_i$, valid for all σ, implies (152).

Since $\mathrm{fix}(\pi)$ is a normal subgroup of $\mathrm{stab}(\pi)$, the quotient group $\mathrm{stab}(\pi)/\mathrm{fix}(\pi)$ is well defined. Moreover, as "$\sim$" induces an equivalence relation on the partition $\pi = \{c_1,\ldots,c_n\}$, we may define $\mathrm{Perm}(\pi)$ as the subgroup of S_k comprising only those elements that permute equivalent cells. Both groups are naturally isomorphic

$$\mathrm{stab}(\pi)/\mathrm{fix}(\pi) \cong \mathrm{Perm}(\pi)\,. \tag{153}$$

We can set up an isomorphism as follows. Use the $\mathrm{fix}(\pi)$ subgroup to permute in each cell c_i the equivalent elements it contains into some lexicographic order. Then cells $c_i, c_{i'}$ are equivalent iff they contain lexicographically ordered strings of equal cardinalities for each "$\sim$" equivalence class. The quotient group permutes equivalent cells while preserving the lexicographic order of the strings. As such it gives one realization of $\mathrm{Perm}(\pi)$ and hence (153). Since $|\mathrm{fix}(\pi)| = |\mathrm{fix}(\nu_0^B)|$ it follows that $|\mathrm{stab}(\pi)| = |\mathrm{Perm}(\pi)||\mathrm{fix}(\nu_0^B)|$. When treating π as a label set for the graphs $T \in \mathcal{T}(B(v),n)$ the automorphism group $\mathrm{Aut}(T)$ is a subgroup of

$\mathrm{Perm}(\pi)$. Lagrange's theorem

$$\frac{|\mathrm{Perm}(B)|}{|\mathrm{fix}(\nu_0^B)||\mathrm{Aut}(T)|} = \frac{|\mathrm{Perm}(B)|}{|\mathrm{stab}(\pi)|}\frac{|\mathrm{Perm}(\pi)|}{|\mathrm{Aut}(T)|} \in \mathbb{N}\,, \tag{154}$$

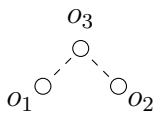
completes the argument. □

We proceed with labeling the dashed graphs $t \in \mathcal{T}_n$ by an abstract n element label set $C = \{c_1, \ldots, c_n\}$. Later on the c_i will be identified with the cells of a set partition in $\mathcal{S}(B(v), n)$, for now the origin of the c_i's is irrelevant. In order to model the equivalence of cells we assume that C carries an equivalence relation "$\sim$" and that a subgroup $\mathrm{Perm}(C)$ of S_n acts by permuting equivalent c_i's. As before, only the open circle vertices ν_0 of $t \in \mathcal{T}_n$ are labeled, technically via the graph of a bijection $\sigma : \nu_0 \to C$. Each graph is referred to as a labeling set (or pairing) and corresponds to a permutation $\sigma \in S_n$, so for $\nu_0 = \{o_1, \ldots, o_n\}$ and $C = \{c_1, \ldots, c_n\}$ we write a labeling set as $\nu_0^\sigma = \{(o_i, c_{\sigma(i)}) : i = 1, \ldots, n\}$, by slight abuse of notation. For fixed C we now consider the set of all pairings

$$\nu_0^C = \{\nu_0^\sigma : \sigma \in S_n\}\,, \quad |\nu_0^C| = n!\,. \tag{155}$$

Recall that an unlabeled graph $t \in \mathcal{T}_n$ may be written as $t = (\nu_0 \cup \nu_1, \epsilon)$, for one of its labeled counterparts we write $T = (\nu_0^\sigma \cup \nu_1, \epsilon)$. As σ runs through S_n the set of labeled dashed graphs generated is denoted by $\mathcal{T}_n^C$.

The product group $\mathrm{Aut}(t) \times \mathrm{Perm}(C) : \nu_0^C \to \nu_0^C$ acts termwise on the elements of ν_0^σ: for $(g, h) \in \mathrm{Aut}(t) \times \mathrm{Perm}(C)$ and $\nu_0^\sigma = \{(o_i, c_{\sigma(i)}) : i = 1, \ldots, n\}$ define $(g, h)(o_i, c_{\sigma(i)}) := \big(g(o_i), h(c_{\sigma(i)})\big)$. We note that two distinct labeling sets $\nu_0^{\sigma_1}, \nu_0^{\sigma_2} \in \nu_0^C$ with $\sigma_1 \neq \sigma_2$ can correspond to the same labeled $T \in \mathcal{T}_n^C$. This occurs if there is an element of $\mathrm{Aut}(t) \times \mathrm{Perm}(C)$ that maps between the labeling sets. As an illustration consider $t \in \mathcal{T}_3$ with open circle vertex set $\nu_0 = \{o_1, o_2, o_3\}$

t 

(156)

With labels $C = \{c_1, c_2, c_3\}$ two distinct labeling sets are $\nu_0^{\sigma_1} = \big\{(o_1, c_1), (o_2, c_2), (o_3, c_3)\big\}$ and $\nu_0^{\sigma_2} = \big\{(o_1, c_2), (o_2, c_1), (o_3, c_3)\big\}$, and the resulting labeled graphs T_1 and T_2 are shown

in (157). On inspection it is clear that T_1 and T_2 are the same labeled graph as one can be mapped into the other by interchanging o_1 and o_2.

$$T_1 \quad \begin{array}{ccc} & (o_3,c_3) & \\ \circ & & \circ \\ (o_1,c_1) & & (o_2,c_2) \end{array} \qquad T_2 \quad \begin{array}{ccc} & (o_3,c_3) & \\ \circ & & \circ \\ (o_1,c_2) & & (o_2,c_1) \end{array} \tag{157}$$

Generally, labeling sets related by the above action of $\mathrm{Aut}(t) \times \mathrm{Perm}(C)$ give rise to the same labeled graph. This underlies the following

Lemma 3.4.3. *Let $t \in \mathcal{T}_n$ be an unlabeled graph and $C = \{c_1, \ldots, c_n\}$ be a set of distinct labels equipped with an equivalence relation "$\sim$". Let Perm(C) be the subgroup of S_n that permutes equivalent c_i's, and let $\mathcal{T}_n^C(t)$ be the set of all topologically distinct labeled dashed graphs obtained by labeling t with C. Then:*

$$\sum_{T \in \mathcal{T}_n^C(t)} \frac{|\mathrm{Perm}(C)|}{|\mathrm{Aut}(T)|} = \frac{n!}{|\mathrm{Aut}(t)|}, \tag{158}$$

i.e. this sum is independent of the equivalence relation "$\sim$" on C.

Proof. We consider the orbit $\mathrm{orb}(\nu_0^\sigma)$ of some $\nu_0^\sigma \in \nu_0^C$ under the action of $\mathrm{Aut}(t) \times \mathrm{Perm}(C)$. By the comment after (157) the orbit is the subset of ν_0^C whose elements correspond to the same labeled graph T. Hence there exists a bijection between labeled graphs in $\mathcal{T}_n^C(t)$ and equivalence classes in $\nu_0^C/[\mathrm{Aut}(t) \times \mathrm{Perm}(C)]$, *i.e.* orbits. The orbits are disjoint and their union is ν_0^C. A sum over $T \in \mathcal{T}_n^C(t)$ may be reexpressed as a sum over orbits $[\nu_0^\sigma] \in \nu_0^C/[\mathrm{Aut}(t) \times \mathrm{Perm}(C)]$.

Next we claim that $\mathrm{Aut}(T)$ for a labeled $T \in \mathcal{T}_n^C(t)$ is isomorphic to some subgroup $\mathrm{Aut}(t) \times \mathrm{Perm}(C)$. Suppose an element of $\mathrm{Aut}(T)$ permutes two labeled vertices (o, c) and (o', c') while preserving adjacency. This is possible iff there is a $g \in \mathrm{Aut}(t)$ that exchanges v, v', *and* there is a $h \in \mathrm{Perm}(C)$ that exchanges c, c'. For a labeling set ν_0^σ corresponding to T, then $(g \times h)(\nu_0^\sigma) = \nu_0^\sigma$. Conversely, suppose there is an element of $\mathrm{Aut}(t) \times \mathrm{Perm}(C)$ that leaves ν_0^σ invariant. This is a permutation of the pairs in ν_0^σ labeling T that preserves adjacency in t, and so there is a corresponding element in $\mathrm{Aut}(T)$. Thus $\mathrm{Aut}(T)$ is isomorphic

to the subgroup $\mathrm{stab}(\nu_0^\sigma)$ of $\mathrm{Aut}(t) \times \mathrm{Perm}(C)$ that leaves any labeling set ν_0^σ corresponding to T invariant.

The stabilizer subgroups of two elements $\nu_0^\sigma, \nu_0^{\sigma'}$ of the same orbit are related by conjugation with the group element linking them. In particular, $|\mathrm{stab}(\nu_0^\sigma)| = |\mathrm{stab}(\nu_0^{\sigma'})|$, for $\nu_0^\sigma, \nu_0^{\sigma'} \in \mathrm{orb}(\nu_0^\sigma)$. We may write

$$\sum_{T \in \mathcal{T}_n^C(t)} \frac{|\mathrm{Perm}(C)|}{|\mathrm{Aut}(T)|} = \sum_{[\nu_0^\sigma] \in \nu_0^C / [\mathrm{Aut}(t) \times \mathrm{Perm}(C)]} \frac{|\mathrm{Perm}(C)|}{|\mathrm{stab}(\nu_0^\sigma|}. \tag{159}$$

The orbit-stabilizer theorem implies $|\mathrm{Aut}(t) \times \mathrm{Perm}(C)| = |\mathrm{stab}(\nu_0^\sigma)||\mathrm{orb}(\nu_0^\sigma)|$, i.e. $|\mathrm{Perm}(C)|/|\mathrm{stab}(\nu_0^\sigma)| = |\mathrm{orb}(\nu_0^\sigma)|/|\mathrm{Aut}(t)|$. Thus

$$\sum_{T \in \mathcal{T}_n^C(t)} \frac{|\mathrm{Perm}(C)|}{|\mathrm{Aut}(T)|} = \frac{1}{|\mathrm{Aut}(t)|} \sum_{[\nu_0^\sigma] \in \nu_0^C / [\mathrm{Aut}(t) \times \mathrm{Perm}(C)]} |\mathrm{orb}(\nu_0^\sigma)| = \frac{|\nu_0^C|}{|\mathrm{Aut}(t)|}\,, \tag{160}$$

as claimed. □

We proceed to a variant of Lemma 3.4.3 where the equivalence relation on C is compatible with an integer grading $d : C \to \mathbb{N}^n$. Each element of the label set $C = \{c_1, \ldots, c_n\}$ is assigned an integer $d(c_i) \in \mathbb{N}$. The range $d(C) = \{d(c_1), \ldots, d(c_n)\}$ will in general be a multiset $D_n = \{d_1^{s_1}, \ldots, d_n^{s_n}\}$, with $\sum_{i=1}^n s_i = n$, $s_i \in \mathbb{N}_0$. If C is used to label some $t \in \mathcal{T}_n$, the weight assignment to its open circle vertices will by (112), (114) depend only on the valency of the $o \in \nu_0$ and some integers which we will now draw drom the range $d(C)$. To this end we extend the ddeg function in (112) to the labeled vertices $(o_i, c_{\sigma(i)})$ by $\mathrm{ddeg}(o_i, c_{\sigma(i)}) = |o_i| + d(c_{\sigma(i)})$. In other words, the sum $|o_i| + d(c_{\sigma(i)})$ is viewed as an instance of (112) where the integers arise from the degrees of the labeling set. This carries over to $\mathrm{ddeg}\nu_0^\sigma := \{\mathrm{ddeg}(o_i, c_{\sigma(i)}) : i = 1, \ldots, n\}$ and we define

$$\begin{aligned} \mathcal{T}^C(\rho_n) &:= \{T \in \mathcal{T}_n^C(t) : \mathrm{ddeg}\nu_0^\sigma = \rho_n\}\,, \\ \nu_0(\rho_n) &:= \{\nu_0^\sigma \in \nu_0^C : \mathrm{ddeg}\nu_0^\sigma = \rho_n\}\,, \end{aligned} \tag{161}$$

for some fixed $\rho_n \in \rho(t, d(C))$ in the range of the ddeg function

$$\rho(t, d(C)) := \{\mathrm{ddeg}\nu_0^\sigma : \sigma \in S_n\}\,. \tag{162}$$

By the weight assigments (114) all $T \in \mathcal{T}^C(\rho_n)$ have the same $\mu(T)$. Equivalently, elements ν_0^σ, $\nu_0^{\sigma'}$ of the same orbit in $\nu_0^C/[\mathrm{Aut}(t) \times \mathrm{Perm}(C)]$, have the same ρ_n and hence lie in the same $\nu_0(\rho_n)$. Clearly, $\mathcal{T}_n^C(t)$ is partitioned by $\mathcal{T}^C(\rho_n)$ as ρ_n runs through $\rho(t, d(C))$.

Lemma 3.4.4. *Let $t \in \mathcal{T}_n$ be an unlabeled graph and $C = \{c_1, \ldots, c_n\}$ be a set of distinct labels equipped with a grading $d : C \to \mathbb{N}^n$ and a compatible equivalence relation "$\sim$", i.e. $c_i \sim c_j$ only if $d(c_i) = d(c_j)$. Then:*

$$\sum_{T \in \mathcal{T}^C(\rho_n)} \frac{|\mathrm{Perm}(C)|}{|\mathrm{Aut}(T)|} = \frac{|\nu_0(\rho_n)|}{|\mathrm{Aut}(t)|}\,, \tag{163}$$

i.e. the sum is independent of the equivalence relation "$\sim$" on C.

Proof. As noted in the proof of Lemma 3.4.3, there is a bijection between the labeled graphs in $\mathcal{T}_n^C(t)$ and the orbits in $\nu_0^C/[\mathrm{Aut}(t) \times \mathrm{Perm}(C)]$. Therefore we may write

$$\begin{aligned}\sum_{T \in \mathcal{T}(t,\rho_n)} \frac{|\mathrm{Perm}(C)|}{|\mathrm{Aut}(T)|} &= \sum_{[\nu_0^\sigma] \in \nu_0(\rho_n)/[\mathrm{Aut}(t) \times \mathrm{Perm}(C)]} \frac{|\mathrm{Perm}(C)|}{|\mathrm{stab}(\nu_0^\sigma)|} \\ &= \frac{1}{|\mathrm{Aut}(t)|} \sum_{[\nu_0^\sigma] \in \nu_0(\rho_n)/[\mathrm{Aut}(t) \times \mathrm{Perm}(C)]} |\mathrm{orb}(\nu_0^\sigma)| = \frac{|\nu_0(\rho_n)|}{|\mathrm{Aut}(t)|}.\end{aligned} \tag{164}$$

In the first identity the constancy of ρ_n within orbits entered, in the second the orbit-stabilizer theorem was used as in the proof of Lemma 3.4.3. The elements of $\nu_0(\rho_n)$ depend on the grading but not on the specific equivalence relation "$\sim$" compatible with it. □

We now return to the graph rule, where the label set C originates from partitioning the vertex set B into n cells. We adopt the equivalence class setting from Proposition 3.4.1: given a vertex set $B = \{b_1, \ldots, b_I\}$ of I distinct elements its n-cell set partitions $\{c_1, \ldots, c_n\} \in \mathcal{S}(B, n)$ are formed. The cardinality $|\mathcal{S}(B, n)| = S(I, n)$ is the second Stirling number. We stipulate the existence of an equivalence relation "$\sim$" on B, and take $\mathrm{Perm}(B)$ to permute equivalent elements of B. An action $\mathrm{Perm}(B) : \mathcal{S}(B, n) \to \mathcal{S}(B, n)$ is induced, and we write $\mathrm{orb}(\pi)$ for the orbit of $\pi \in \mathcal{S}(B, n)$ under $\mathrm{Perm}(B)$. Observe that for given $\pi \in \mathcal{S}(B, n)$, all elements of $\mathrm{orb}(\pi)$ correspond to the same label set C. We omit a formal proof and instead present an illustrative example: let $B = \{b_1, b_2, b_3, b_4, b_5\}$, with $b_1 \sim b_2$. The partitions $\pi_1 = \big\{\{b_1, b_4\}, \{b_2, b_3, b_5\}\big\}$ and $\pi_2 = \big\{\{b_2, b_4\}, \{b_1, b_3, b_5\}\big\}$ are distinct, but they correspond

to the same label set C by virtue of $b_1 \sim b_2$. We define $\bar{\mathcal{S}}(B,n) := \mathcal{S}(B,n)/\mathrm{Perm}(B)$, the set of distinct label sets C.

Lemma 3.4.5. *Let $B = \{b_1, \ldots, b_I\}$ be a set of distinct vertices equipped with an equivalence relation "$\sim$", and let $\mathrm{Perm}(B)$ be the subgroup of S_I that permutes equivalent vertices. For given $t \in \mathcal{T}_n$ let $\overline{\mathcal{T}}_n^B(t)$ be the set of topologically distinct labeled dashed graphs obtained by labeling t with $C \in \bar{\mathcal{S}}(B,n)$. Then:*

$$\sum_{T \in \overline{\mathcal{T}}_n^B(t)} \frac{|\mathrm{Perm}(B)|}{\mathrm{Sym}(T)} = S(I,n) \frac{n!}{|\mathrm{Aut}(t)|}\,. \tag{165}$$

Proof. We may trivially rewrite the left hand side of (165)

$$\sum_{T \in \overline{\mathcal{T}}_n^B(t)} \frac{|\mathrm{Perm}(B)|}{\mathrm{Sym}(T)} = \sum_{C=[\pi] \in \mathcal{S}(B,n)/\mathrm{Perm}(B)} \sum_{T \in \mathcal{T}_n^C} \frac{|\mathrm{Perm}(B)|}{\mathrm{Sym}(T)}. \tag{166}$$

From (154) we know

$$\frac{|\mathrm{Perm}(B)|}{\mathrm{Sym}(T)} = \frac{|\mathrm{Perm}(B)|}{|\mathrm{stab}(\pi)|} \frac{|\mathrm{Perm}(C)|}{|\mathrm{Aut}(T)|}, \tag{167}$$

where $\mathrm{stab}(\pi)$ is the subgroup of $\mathrm{Perm}(B)$ leaving $\pi \in \mathcal{S}(B,n)$ invariant. It follows from the definition of $\mathcal{S}(B,n)/\mathrm{Perm}(B)$ that if $\pi_1, \pi_2 \in \mathrm{orb}(\pi)$ then $|\mathrm{stab}(\pi_1)| = |\mathrm{stab}(\pi_2)|$. Combining successively (167), Lemma 3.4.3, and the orbit-stabilizer theorem gives the assertion:

$$\begin{aligned} \sum_{C=[\pi] \in \mathcal{S}(B,n)/\mathrm{Perm}(B)} \sum_{T \in \mathcal{T}_n^C} \frac{|\mathrm{Perm}(B)|}{\mathrm{Sym}(T)} &= \sum_{C=[\pi] \in \mathcal{S}(B,n)/\mathrm{Perm}(B)} \left(\frac{|\mathrm{Perm}(B)|}{|\mathrm{stab}(\pi)|} \sum_{T \in \mathcal{T}_n^C} \frac{|\mathrm{Perm}(C)|}{|\mathrm{Aut}(T)|} \right) \\ &= \frac{n!}{|\mathrm{Aut}(t)|} \sum_{[\pi] \in \mathcal{S}(B,n)/\mathrm{Perm}(B)} |\mathrm{orb}(\pi)| = \frac{n!}{|\mathrm{Aut}(t)|} S(I,n). \end{aligned} \tag{168}$$

□

Note that Lemma 3.4.5 is the counterpart of Lemma 3.4.3 for C induced by set partitions. Similarly, Proposition 3.4.1 is the counterpart of Lemma 3.4.4. Instead of holding C fixed we take it to range over all $C \in \overline{\mathcal{S}}(B, D_n)$, as defined before Proposition 3.4.1. Indicating all dependencies in the notation we set

$$\begin{aligned} \overline{\mathcal{T}}^B(t, D_n, \rho_n) &:= \bigcup_{C \in \overline{\mathcal{S}}(B,D_n)} \mathcal{T}^C(\rho_n) \\ &= \{T \in \mathcal{T}_n^B(t) : \mathrm{ddeg}\nu_0^\sigma = \rho_n\,,\ \nu_0^\sigma \in \nu_0^C,\ C \in \overline{\mathcal{S}}(B, D_n)\}\,. \end{aligned} \tag{169}$$

Proof of Proposition 3.4.1. We begin as in the proof of Lemma 3.4.5 and rewrite the left hand side of (150) as

$$\sum_{T\in\overline{\mathcal{T}}^{B}(t,D_n,\rho_n)}\frac{|\mathrm{Perm}(B)|}{\mathrm{Sym}(T)}=\sum_{C=[\pi]\in\mathcal{S}(B,D_n)/\mathrm{Perm}(B)}\sum_{T\in\mathcal{T}^{C}(\rho_n)}\frac{|\mathrm{Perm}(B)|}{\mathrm{Sym}(T)}$$
$$=\sum_{C=[\pi]\in\mathcal{S}(B,D_n)/\mathrm{Perm}(B)}\Bigg(\frac{|\mathrm{Perm}(B)|}{|\mathrm{stab}(\pi)|}\sum_{T\in\mathcal{T}^{C}(\rho_n)}\frac{|\mathrm{Perm}(C)|}{|\mathrm{Aut}(T)|}\Bigg). \tag{170}$$

To the subsum in round brackets we apply Lemma 3.4.4 to obtain

$$\sum_{T\in\overline{\mathcal{T}}^{B}(t,D_n,\rho_n)}\frac{|\mathrm{Perm}(B)|}{\mathrm{Sym}(T)}=\frac{|\nu_0(\rho_n)|}{|\mathrm{Aut}(t)|}\sum_{[\pi]\in\mathcal{S}(B,D_n)/\mathrm{Perm}(B)}\frac{|\mathrm{Perm}(B)|}{|\mathrm{stab}(\pi)|}, \tag{171}$$

using that $|\nu_0(\rho_n)|$ is independent of equivalence relation on $C=[\pi]$. On account of the orbit-stabilizer theorem $|\mathrm{Perm}(B)|/|\mathrm{stab}(\pi)|=|\mathrm{orb}(\pi)|$ the sum over $[\pi]$ produces the cardinality of the set $\mathcal{S}(\{b_1,\ldots,b_I\},D_n)$, i.e. $P(D(v),D_n)$ and establishes (150). Its right hand side is manifestly independent of the (degree compatible) equivalence relation "$\sim$" on B. □

3.5 Conclusions

Motivated by the widespread use of the FRG equation (77) we formulated a program for its graph theoretical solution. Subject to ultralocal initial conditions (77) can be replaced by the iteratively soluble (79) producing a long range hopping expansion (LRH) for $\Gamma_\kappa=\Gamma_0+\sum_{l\geq 1}\kappa^l\Gamma_l$, from which a solution Γ_k of (77) can be obtained by substitution, $\Gamma_k=\Gamma_\kappa|_{\ell\to\ell(k)}$. As the iteration of (511), or its equivalent mixed form (98), is only feasible to moderate orders we formulated graph rules for the direct evaluation of an arbitrary order Γ_l. The derivation, computational test, and proof of these graph rules constitute the main result of this chapter.

By the results of Section 3.4 the subsums over vertex labeled trees $T\in\mathcal{T}(B(v),n)$ with fixed weight $\mu(T)$ have a combinatorial meaning in terms of the number of integer labeled tree graphs of the same topology as T. The graph rule could therefore optimized once explicit results for the number of set partitions $P(D(v),D_n)$ are available; see [33] for some related

results.

The construction so far only holds in the formal series sense. Guided by a variety of convergence results for hopping expansions in the literature (see [18, 85, 54] and the references therein) we expect that the LRH expansion for Γ_κ has finite radius of convergence under natural conditions. From a computational perspective it would also be desirable to identify subclasses of one-line irreducible graphs that can be analytically summed and lead to controlled approximate solutions of (77), replacing the traditional ad-hoc Ansätze.

4.0 Critical Behavior of the Hopping Expansion from the Functional Renormalization Group

4.1 Introduction

The functional renormalization group (FRG) has become one of the most widely and fruitfully used techniques in quantum many body physics, and is now applied to areas as diverse as quantum gravity, particle physics, and solid state physics [63, 104, 82]. The FRG is a reformulation of quantum field theory that focusses on the non-linear response of functionals to a scale dependent mode modulation introduced by replacing the bare action $S[\chi]$ with $S[\chi] + \frac{1}{2}\chi \cdot R_k \cdot \chi$ in the functional integral. The regulator kernel R_k supresses low energy modes and vanishes at $k = 0$, such that the scale k smoothly interpolates between the bare theory and the renormalized theory. Modern formulations focus on the Legendre effective action Γ_k, whose flow satisfies

$$\partial_k \Gamma_k[\phi] = \frac{1}{2}\mathrm{Tr}\big\{\partial_k R_k[\Gamma_k^{(2)} + R_k]^{-1}\big\}\,. \tag{172}$$

The versatility of the flow equation (172) is partly due to its kinematical nature; dynamical information is injected solely through initial conditions. As a consequence, fully non-perturbative results require some such initial conditions. An especially good choice are ultralocal initial conditions as they can, in a lattice formulation, be computed exactly from single site integrals [70]. A solution of (172) with such initial data, if feasible, will emulate a linked cluster or hopping expansion but with a scale dependent long-ranged interaction

$$S[\chi] = \sum_x s[\chi_x] + \frac{\kappa}{2}\sum_{x,y} \chi_y \ell_{xy}(k)\chi_x\,. \tag{173}$$

For definiteness we consider here a self-interacting, one-component, scalar field theory on a D-dimensional hypercubic lattice (identified with $\mathbb{Z}^D$) in a dimensionless formulation. Then, $s : \mathbb{R} \to \mathbb{R}$ is a real even function bounded from below that collects all terms referring to a single site. The hopping parameter $\kappa > 0$ is a dimensionless combination of the original

mass, the coupling parameters, and the lattice spacing. A fundamental lattice action has the form (173) with a k-independent ℓ_{xy} that connects only nearest neighbors. In order to relate (172) to a hopping expansion we take κ itself as the control parameter and replace (172) by

$$\partial_\kappa \Gamma_\kappa = \frac{1}{2} \sum_{x,y} \ell_{xy} \big[\Gamma^{(2)}_\kappa + \kappa \ell\big]^{-1}_{xy}, \quad \Gamma_\kappa[\phi] = \Gamma_0[\phi] + \sum_{l \geq 2} \kappa^l \Gamma_l[\phi]\,. \tag{174}$$

Here $\Gamma_0[\phi] = \sum_x \gamma(\phi_x)$, where γ and its derivatives γ_n are computable at a single site x from s only. The $O(\kappa)$ term vanishes, $\Gamma_2[\phi] = -\frac{1}{4} \sum_{x,y} (\ell_{xy})^2 \gamma_2(\phi_x)^{-1} \gamma_2(\phi_y)^{-1}$, and all Γ_l, $l \geq 3$, are then determined recursively. The direct recursion turns out to become intractable beyond $O(\kappa^6)$, say. However, in the previous chapter we presented a closed graph theoretical solution of the recursion that yields Γ_l for any $l \geq 1$. Importantly, the series in (174) can be expected to have finite radius of convergence $\kappa < \kappa_c$, at least as far as the associated vertex functions are concerned [85]. Once the series (174) has been constructed, an in principle exact solution of (172)'s lattice counterpart arises simply by substitution, $\Gamma_k = \Gamma_\kappa|_{\ell \mapsto \ell(k)}$, for suitable $\ell(k)$ playing the role of R_k. This differs from the standard uses of the FRG [63, 104, 82] in the way initial conditions are imposed: R_k is chosen such that $\Gamma_{k_0}[\phi]$, for some finite $k = k_0$, is (up to kinematical factors) determined by the above $\Gamma_0[\phi] = \sum_x \gamma(\phi_x)$. In overview, we propose to use the graph rule of Chapter 3 for the computation of vertex (and other correlation) functions but determine bulk quantities from the FRGs (172), (174).

This chapter is based on [8].

4.2 Critical behavior from the LPA's unstable manifold

For the hopping expansion the locus of infinite correlation length (approached from the symmetric phase) is deemed to coincide with the radius of convergence κ_c of the (two-point and then all other) susceptibilities. Traditionally, κ_c has been estimated by pushing their hopping expansion to high orders, at considerable effort. Our proposed alternative rests on two simple observations: (i) any bulk quantity other than a susceptibility should give the same κ_c, in particular Γ_κ for constant field (identified with the lattice average) should be a

legitimate choice. (ii) For $\kappa < \kappa_c$, specialization to constant fields and resummation in (174) are commuting operations. The FRG (172) specialized to constant fields (up to kinematical factors) is known as the Local Potential Approximation (LPA), or its modified version LPA' (see [63]). On general grounds, the relation between the bare and renormalized parameters can be found by injecting initial data (determined by the bare parameters) at the ultralocal scale $k = k_0$, and running the flow equation for (truncations of) Γ_k to the fixed point at $k \approx 0$. This yields the correlated values of the bare parameters in the action tuned to ensure that $\Gamma[\phi]$ is based on the fixed point, i.e. the unstable manifold of the fixed point in question. In summary, one should be able to determine κ_c from the unstable manifold of the LPA (or LPA') approximation to the FRG (172).

Explicitly, the following LPA ansatz $\Gamma_k[\phi_0] = a^D \sum_x \{-\frac{1}{2}\phi_0(x)(\Delta\phi_0)(x) + U_k(\phi_0(x))\}$, is taken as the starting point, where Δ is the lattice Laplacian and a the lattice spacing. The flow equation (172) then specializes to

$$\partial_k U_k(\phi_0) = \frac{1}{2}\int_{-\pi/a}^{\pi/a} \frac{d^D p}{(2\pi)^D} \frac{\partial_k R_k(p)}{\hat{p}^2 + R_k(p) + U_k''(\phi_0)}\,, \tag{175}$$

where the k differentiation is at fixed ϕ_0 and $\hat{p}^2 = \frac{4}{a^2}\sum_j \sin^2 \frac{p_j a}{2}$. Next we fix lattice units ($a = 1$) and choose $R_k(p)$ to be the lattice step function $R_k(p) = (k^2 - \hat{p}^2)\theta(k^2 - \hat{p}^2)$. Then

$$k\partial_k U_k(\phi_0) = \frac{k^2\,\mathrm{Vol}(k)}{k^2 + U_k''(\phi_0)}\,, \quad \mathrm{Vol}(k) := \int_{-\pi}^{\pi} \frac{dp}{(2\pi)^D}\,\theta(k^2 - \hat{p}^2)\,. \tag{176}$$

The above flow equations and the fields have been dimensionful, and as such they do not lend themselves to a fixed point analysis. In particular the dimensionful LPA potential $U_k(\phi_0)$ will not itself reach a fixed point, but rather exhibit a characteristic scaling behavior. To proceed we transition to a dimensionless LPA formulation by rescaling both the field and potential,

$$V_k(\phi) := \frac{1}{\mu_D k^D} U_k(\phi_0(\phi))\,, \quad \phi_0(\phi) := k^{\frac{D-2}{2}}\sqrt{\mu_D}\,\phi\,, \quad \mu_D := \frac{1}{(4\pi)^{D/2}\Gamma(\frac{D}{2}+1)}\,. \tag{177}$$

The new potential $V_k(\phi)$ is a dimensionless function of the dimensionless field ϕ. The constants are adjusted such that only the dimensionless volume function $\mathrm{vol}(s) := \frac{\mathrm{Vol}(k_0 s)}{\mu_D k_0^D s^D}$, $0 \le s := k/k_0 \le 1$, $k_0 := \sqrt{4D}$, occurs. It is determined numerically, and is roughly

bell shaped with a maximum of $O(1)$. The normalizations are such that $\mathrm{vol}(0) = 1$ and $\mathrm{vol}(1) = 1/\mu_D k_0^D$.

The dimensionful flow equation (176) translates into

$$s\partial_s V_s(\phi) = -DV_s(\phi) + \frac{D-2}{2}\phi V_s'(\phi) + \frac{\mathrm{vol}(s)}{1+V_s''(\phi)}\,. \tag{178}$$

In this form one can now search meaningfully for a $s \to 0$ fixed point potential solving

$$0 = -DV_*(\phi) + \frac{D-2}{2}\phi V_*'(\phi) + \frac{1}{1+V_*''(\phi)}\,. \tag{179}$$

To proceed, insertion of the Taylor series $V_s(\phi) = \sum_{i\geq 0}\frac{g_{2i}(s)}{(2i)!}\phi^{2i}$ into (178) produces the beta functions for the couplings $g_{2i}(s)$,

$$\begin{aligned} s\partial_s g_{2i} &= \beta_{2i}(g_2,\ldots,g_{2i+2})\,, \quad i\geq 1\,,\\ \beta_2 &= -2g_2 - \frac{\mathrm{vol}(s)}{(1+g_2)^2}\,g_4\,, \quad \beta_4 = (D-4)g_4 - \frac{\mathrm{vol}(s)}{(1+g_2)^2}\,g_6 + \frac{6\mathrm{vol}(s)}{(1+g_2)^3}\,g_4^2\,, \end{aligned} \tag{180}$$

etc. Truncating via $g_{2N+2} \equiv 0$ at some order N a closed system of $N+1$ ordinary differential equations (ODEs) arises. The lowest order equation $s\partial_s g_0 = -Dg_0 + \mathrm{vol}(s)/(1+g_2)$ determines g_0 once g_2 is known.

Clearly, the behavior of the dimensionless couplings in the vicinity of the fixed point is instrumental for the critical behavior. The fixed couplings themselves obey a simple recursion relation of the form $g_{2i}^* = -2g_2^*(1+g_2^*)^i P_{i-2}(g_2^*)$, where generally P_n is a polynomial of degree n. The value of g_2^* is constrained by the truncation condition $g_{2N+2}^* = 0$, *i.e.* it is the root of the high order polynomial equation $2g_2^*(1+g_2^*)^{n+1}P_{n-1}(g_2^*) = 0$. In general this equation produces many spurious 'fixed points', but the 'correct' solution can be selected by requiring that its corresponding stability matrix,

$$M(g^*)_{ij} := \left.\frac{\partial\beta_{2i}}{\partial g_{2j}}\right|_{g=g^*}\,, \tag{181}$$

have precisely one negative eigenvalue, conventionally denoted by $-\theta_1$. For $D \geq 3$ one always has a Gaussian fixed point with $-\theta_1 = -2$. In $D = 3$ one finds in addition the Fisher-Wilson fixed point with $-\theta_1 \approx -1.5396$.

The stability matrix M determines the flow pattern in the vicinity of the fixed point.

Writing $\delta g = (\delta g_2, \delta g_4, \ldots, \delta g_{2N})$ for a perturbation about the fixed point g^* and expanding the truncated system (180) to linear order in the perturbation gives $s\partial_s \delta g = M(g^*)\delta g$. The solution of this linearized flow can be written in terms of the eigensystem $(v^{(j)}, -\theta_j)$ of M as

$$\delta g(s) = \sum_{j=1}^{N} c_j v^{(j)} s^{-\theta_j} \,, \tag{182}$$

where the boundary constants $c_1, \ldots, c_N$ are set at some scale $0 < s_0 \ll 1$. For small s and $c_2 \neq 0$ the sum will be dominated by the $j = 1$ term (as $-\theta_1 < 0$) and thus blow up, taking the couplings away from the fixed point. Conversely, the locus of linearized couplings that flow to g^* for $s \to 0$ is characterized by $c_2 = 0$. More intrinsically, there exists a unique linear combination such that

$$a_0 + \sum_{i=1}^{N} a_i \, g_{2i}(s) = \text{const}\, c_2 \, s^{-\theta_1} \,, \quad 0 < s \leq s_0 \ll 1 \,. \tag{183}$$

For $c_2 = 0$ this linear combination describes the "linearized unstable manifold", i.e. the codimension one hyperplane from which the couplings flow into the fixed point. The coefficients of the unstable manifold can be computed analytically for the Gaussian fixed point in $D = 4$, and come out as $a_0 = 0$, $a_i = 1/[2^{i-1}(i-1)!]$, for $1 \leq i \leq N$.

So far no action-specific information has entered. The fixed point, the critical exponents, and the linearized unstable manifold are computable solely in terms of the field content (here: one scalar field), the dimensionality D, the nature of the truncation (here: LPA), and the mode modulator (here: the lattice step function). Action-specific information is in the present setting injected by specifying initial data $g_{2i}(s = 1)$, computed from the ultralocal part of the theory's action.

In order to obtain this intial data, we first note that at any scale k, the Legendre effective action Γ_k in (172) satisfies the functional integro-differential equation

$$e^{-\Gamma_k[\phi_0]} = \int \prod_x d\chi_0(x) e^{-S[\chi_0] - \frac{1}{2}(\phi_0 - \chi_0)\cdot R_k \cdot (\phi_0 - \chi_0) - (\phi_0 - \chi_0)\cdot \frac{\delta \Gamma_k}{\delta \phi_0}} \,, \tag{184}$$

where $S[\chi_0] = \frac{1}{2}\sum_x \big\{ -\chi_0(x)(\Delta\chi_0)(x) + m_0^2 \chi_0(x)^2 + \lambda_0 \chi_0(x)^4/12 \big\}$ is the bare action, and '$\cdot$' denotes a sum over lattice sites. Although this equation cannot in general be solved exactly,

at the ultralocal scale $k_0 = \sqrt{4D}$ where $R_{k_0}(x,y) = k_0^2\delta_{xy} + \Delta_{xy}$, (184) transcribes to

$$e^{-\sum_x U_{k_0}(\phi_0(x))} = \int \prod_x d\chi_0(x) e^{-S_0[\chi_0] - \frac{k_0^2}{2}(\phi_0-\chi_0)\cdot(\phi_0-\chi_0) - (\phi_0-\chi_0)\cdot U'_{k_0}} . \tag{185}$$

Here $S_0[\chi_0]$ is the ultralocal part of the bare action, and U_{k_0} is the effective potential at $k = k_0$. Since all the quantities in (185) are ultralocal, the functional integral factorizes. After transitioning to a dimensionless potential $V_s(\phi)$ viz. (177), and hopping parametrizing the bare action, we obtain the ordinary integro-differential equation satisfied by $V_{s=1}(\phi)$

$$e^{-\mathrm{vol}(1)^{-1}V_{s=1}(\phi)} = \int d\chi e^{-\frac{1-2\lambda-D\kappa}{4D\mathrm{vol}(1)\kappa}\chi^2 - \frac{\lambda}{(4D\mathrm{vol}(1)\kappa)^2}\chi^4 - \frac{1}{2\mathrm{vol}(1)}(\phi-\chi)^2 - \mathrm{vol}(1)^{-1}(\phi-\chi)V'_{s=1}(\phi)} . \tag{186}$$

Inserting the truncation ansatz $V_{s=1}(\phi) = \sum_{i=0}^N \frac{g_{2i}(s=1)}{(2i)!}\phi^{2i}$ into (186) then determines the initial couplings $g_{2i}(s=1)$ as functions of the bare parameters κ, λ via exactly computable single site integrals.

With the initial data known, the integration of the flow equations (180) (truncated at some order N) proceeds as follows. Since the initial data $g_{2i}(s=1)$, $1 \le i \le N$, are prescribed functions of κ, λ, a well-defined evolution via the ODE system will render the $g_{2i}(s) = g_{2i}(s|\kappa,\lambda)$ parametrically dependent on κ, λ for all s for which the evolution is regular. For generic κ, λ the flow will *not* come close to the fixed point; it will do so however once it reaches the linearized unstable manifold at some $0 < s_0 \ll 1$. In a given polynomial approximation of order N one therefore needs to solve

$$a_0 + \sum_{i=1}^N a_i g_{2i}(s_0|\kappa,\lambda) = 0 \quad \Longrightarrow \quad \kappa = \kappa_c(\lambda) . \tag{187}$$

In the present context this will ensure that the flow very nearly reaches the fixed point, with limitations only set by numerical accuracy.

4.3 Results for ϕ^4_3 and ϕ^4_4 and concluding remarks

The above technique has been applied to determine $\kappa_c(\lambda)$ for ϕ^4 theories in both $D = 3$ and $D = 4$. The shooting technique has been implemented in `Mathematica` without

encountering significant obstructions from stiffness for reasonably large N. Related results have been obtained in [20], [21] in a different LPA formulation but without relation to (174) and the hopping expansion's radius of convergence.

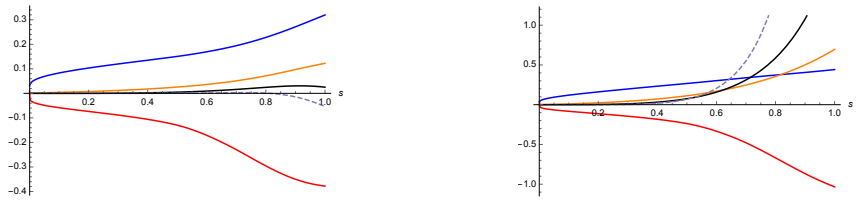
As a proof of principle we first applied the shooting technique in $D=3$, aiming at the Fisher-Wilson fixed point. Since in $D = 3$ the anomalous dimension η is non-zero, the neglection of a wavefunction renormalization constant in the LPA (as opposed to the LPA' ansatz) induces a systematic error. Nevertheless, the comparison of the LPA results with Monte-Carlo data [47] shows reasonable agreement.

λ	$\kappa_{c,MC}$	κ_c	λ	$\kappa_{c,MC}$	κ_c
0.1	0.37341	0.3732	0.9	0.38451	0.3854
0.2	0.3884	0.3882	1.3	0.36522	0.3659
0.4	0.3975	0.3975	1.4	0.36028	0.362
0.7	0.39253	0.3926	1.5	0.3553	0.358
0.8	0.3887	0.3898	2.5	0.3134	0.3149

Table 3: Critical values for ϕ_3^4 theory in $D = 3$. Left, $\kappa_{c,MC}$ from [47] with only significant digits displayed. Right κ_c from LPA at truncation order $N = 20$. The LPA errors are a combination of numerical and estimated truncation effects, only significant digits are displayed. The discrepancy can plausibly be attributed to the neglected anomalous dimension.

In $D = 4$ only the Gaussian fixed point is found. By working with the LPA the $\eta = 0$ contention [90] is probed for self consistency. As an illustration of the shooting technique we depict in Figs. 1(a) and 1(b) the flow of the couplings $g_2(s)$, $g_4(s)$, $g_6(s)$, $g_8(s)$, and $g_{10}(s)$ in the ϕ_4^4 theory towards the Gaussian fixed point. The truncation order is $N = 20$, with κ adjusted at fixed λ such that the $g_{2i}(s_0 = 0.001|\kappa, \lambda)$ satisfy (187), with coefficients $a_0 = 0$, $a_i = 1/[2^{i-1}(i-1)!]$, for $1 \leq i \leq N$.

As noted earlier, the critical line $\kappa_c(\lambda)$ has been previously computed from the radius of convergence of the hopping expansion in [69]. A comparison of our results with the $\kappa_c(\lambda)$ values of Lüscher-Weisz (taken from Table 1 in [69]) is presented in Table 2.



(a) (b)

Figure 4: ϕ_4^4: flow of couplings $g_2(s)$, $g_4(s)$, $g_6(s)$, $g_8(s)$, $g_{10}(s)$ for (a) $(\lambda, \kappa) = (0.48548, 0.2828)$, and (b) $(\lambda, \kappa) = (4.3303, 0.1834)$. `Red`: g_2, `Blue`: g_4, `Orange`: g_6, `Black`: g_8, `Dashed`: g_{10}.

In summary, the critical behavior in the hopping expansion, traditionally set by the radius of convergence [69], [85], can alternatively be obtained simply from the LPA or LPA' approximation to the FRG.

λ	$\kappa_{c,LW}$	$\kappa_c/2$
0	0.1250(1)	0.1250(1)
2.4841×10^{-2}	0.1294(1)	0.12928(3)
3.5562×10^{-2}	0.1308(1)	0.13068(3)
1.3418×10^{-1}	0.1385(1)	0.1381(4)
2.7538×10^{-1}	0.1421(1)	0.1416(4)
4.8548×10^{-1}	0.1418(1)	0.1414(4)
7.7841×10^{-1}	0.1376(1)	0.1374(4)
1.7320	0.1194(1)	0.1190(5)
2.5836	0.1067(1)	0.1066(5)
4.3303	0.09220(9)	0.0917(7)
∞ (LW) or 100 (LPA)	0.07475(7)	0.0722(1)

Table 4: Critical values for ϕ_4^4 theory in $D = 4$. Left, $\kappa_{c,LW}$ from Lüscher-Weisz [69]. Right $\kappa_c/2$ from LPA at truncation order $N = 20$. The errors in the LPA results are a combination of numerical and estimated truncation errors.

5.0 Hadamard States on Friedmann-Lemaître Spacetimes: States of Low Energy

5.1 Introduction

For perturbatively defined quantum field theories on globally hyperbolic spacetimes there is a general consensus that the free state on which perturbation theory is based should be a Hadamard state. By-and-large the Hadamard property is necessary and sufficient for the existence of Wick powers of arbitrary order and hence for the perturbative series to be termwise well-defined at any order, see [61, 36] for recent accounts. On the other hand, Hadamard states are surprisingly difficult to construct concretely [24, 56, 17] even for background spacetimes with some degree of symmetry (other than maximal). The well-known adiabatic iteration [81] has certain characteristics necessary for the Hadamard property to be built in, but is not convergent and cannot be fruitfully extended to small spatial momenta. The iteration can, however, serve as a conduit to establish the existence of states locally indistinguishable from Hadamard states [56].

An important class of backgrounds are generic Friedmann-Lemaître cosmologies, where a construction of exact Hadamard states has become available only relatively recently [80]. These States of Low Energy (SLE) arise by minimizing the Hamiltonian's expectation value *after* averaging with a temporal window function f. The temporal averaging is crucial and avoids the pathologies [41] of the earlier instantaneous diagonalization procedure. The construction of a SLE takes some fiducial solution S of the homogeneous wave equation as a starting point, considers arbitrary Bogoliubov transformations thereof, and then minimizes the temporal average of the energy with respect to them. Olbermann's theorem [80] states that (for a massive free quantum field theory on a Friedmann-Lemaître background) the minimizing solution $T\,[S]$ gives rise to an exact Hadamard state. For given S the minimizer $T\,[S]$ is unique up to a phase.

Here we show that the SLE have a number of bonus properties that make them mathematically even more appealing and which also render them good candidates for vacuum-like

states in a pre-inflationary period. Specifically, we show that for a given temporal averaging function f:

(a) The SLE two-point function $W[S]$ based on a fiducial solution S is a Bogoliubov invariant, $W[aS + bS^*] = W[S]$, with $a, b \in \mathbb{C}$, $|a|^2 - |b|^2 = 1$. Hence $W[S]$ is independent of the choice of fiducial solution S.

(b) The minimization over Bogoliubov parameters relative to a given S can be replaced by a minimization over initial data, without reference to any fiducial solution. The resulting expression for the SLE solution $T[\Delta]$ is fully determined by the (Bogoliubov invariant and state independent) commutator function Δ, making manifest the uniqueness of the SLE. The minimization over initial data has a natural interpretation in the Schrödinger picture.

(c) The SLE solution admits a *convergent* series expansion in powers of the (modulus of the) spatial momentum, both for massive and for massless theories.

(d) In the massless case the leading infrared behavior is Minkowski-like for *all* cosmological scale factors. This provides a new cure for the long standing infrared divergences in Friedmann-Lemaître backgrounds with accelerated expansion [37].

(e) The modulus square of an SLE solution admits an asymptotic expansion in inverse odd powers of the (modulus of the) spatial momentum, which is *independent of the window function* f. The coefficients of the expansion are *local*, recursively computable, and generalize the heat kernel coefficients. The asymptotics of the phase is governed by single integrals of the same coefficients. This short cuts the detour via the adiabatic expansion.

Since linearized cosmological perturbations are described by massless free fields, the property (d) renders SLE a legitimate choice for a vacuum-like state in the early universe. Specifically, we argue that within the standard paradigm (classical Friedmann-Lemaître backgrounds with selfinteracting scalar field) inflation must have been preceded by a period of non-accelerated expansion, for which the type with kinetic energy domination is mathematically preferred. The occurrence of the Bunch-Davies vacuum at the onset of inflation then requires extreme fine tuning. In contrast, postulating a SLE for the primordial vacuum in

the pre-inflationary phase is shown to automatically produce a qualitatively realistic power spectrum at the end of inflation.

This chapter is organized as follows. After introducing the SLE in the Heisenberg and the Schrödinger pictures we establish properties (a) and (b) in Sections 5.2.2 and 5.2.3, respectively. The existence of a convergent small momentum expansion is shown in Section 5.3.1, with the massless case detailed in Section 5.3.2. For large momentum, the existence of the WKB type expansion governed by generalized heat kernel coefficients is shown in Section 5.4. Next, we study the viability of massless SLE as pre-inflationary vacua in Section 5.5. Finally, in Section 5.6 we generalize the SLE construction to a one-parameter family of exact Hadamard states.

This chapter is based on [7].

5.2 SLE in the Heisenberg and Schrödinger pictures

A State of Low Energy (SLE) was originally defined in the Heisenberg picture by minimizing with respect to Bogoliubov parameters relating the corresponding solution of the wave equation to a reference solution S. As such, the SLE construction depends on the reference solution. Here we show that the SLE two-point function (which specifies the state completely) is independent of S. Next, the energy functional in the Schrödinger picture is naturally regarded as a function of the wave function's initial data. By minimizing over initial data an alternative explicit expression for the SLE is obtained, which depends only on the (Bogoliubov invariant and state independent) commutator function.

5.2.1 Homogeneous pure quasifree states in Heisenberg and Schrödinger pictures

Throughout, the background geometry will be a $1+d$ dimensional, spatially flat Friedmann-Lemaître (FL) cosmology with line element

$$ds^2 = -\bar{N}(t)^2 dt^2 + a(t)^2 \delta_{ij} dx^i dx^j \,, \tag{188}$$

where $\bar{N} : \mathbb{R}_+ \to \mathbb{R}_+$ is the lapse function, $a : \mathbb{R}_+ \to \mathbb{R}_+$ is the cosmological scale factor, and $x^i, i = 1, \ldots, d$ are adapted spatial coordinates. The form of the line element (188) is preserved under $\mathrm{Diff}[t_i, t_f] \times \mathrm{ISO}(d)$ transformations, where $\mathrm{Diff}[t_i, t_f]$ are endpoint preserving reparameterizations of some time interval $[t_i, t_f]$, $0 < t_i < t_f < \infty$, and the Euclidean group $\mathrm{ISO}(d)$ acts via global spatial diffeomorphisms connected to the identity. On this background we consider a scalar field $\chi : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}$, which is minimally coupled and initially selfinteracting with potential $U(\chi)$. Under the temporal reparameterizations $a(t)$ and $\chi(t, x)$ transform as scalars, while $\bar{N}(t)$ and $\bar{n}(t) := \bar{N}(t)/a(t)^d$ are temporal densities, $\bar{n}'(t') = \bar{n}(t)/|\partial t'/\partial t|$, etc.. This is such that $\int_{t_i}^{t_f} dt \bar{N}(t) a(t)^p = \int_{t_i}^{t_f} dt\, \bar{n}(t) a(t)^{p+d}$ is invariant for any p. Next, we expand the minimally coupled scalar field action on $[t_i, t_f] \times \mathbb{R}^d$ around a spatially homogeneous background scalar $\varphi(t)$ to quadratic order in the fluctuations $\phi(t, x) := \chi(t, x) - \varphi(t)$. This gives a leading term $\bar{S}^\varphi$ (multiplied by a spatial volume term) whose field equation is one of the evolution equations for a FL cosmology. For $\varphi(t)$ solving it (with prescribed $a(t)$) the term linear in the ϕ reduces to a boundary term and may be omitted. The quadratic piece reads

$$S^\phi = \frac{1}{2} \int_{t_i}^{t_f} dt \int_\Sigma dx \left\{ \frac{1}{\bar{n}(t)} (\partial_t \phi)^2 - \bar{n}(t) a(t)^{2d} U''(\varphi) \phi^2 - \bar{n}(t) a(t)^{2d-2} \partial_i \phi \delta^{ij} \partial_j \phi \right\}. \quad (189)$$

So far, φ is for prescribed $a(t)$ a solution of $\partial_t(\bar{n}^{-1}\partial_t\varphi) + \epsilon_g \bar{n} a^{2d} U'(\varphi) = 0$, but $a(t)$ itself is unconstrained. As far as the homogeneous background is concerned one could now augment the missing gravitational dynamics by the other FL field equations. This would turn $a(t), \varphi(t)$ into a solution of the Einstein equations and classical backreaction effects would be taken into account in the homogeneous sector. The standard "Quantum Field Theory (QFT) on curved background" viewpoint, on the other hand, treats the geometry as external, in which case (189) adheres to the minimal coupling principle only if $U''(\varphi) = m_0^2$ is identified with a constant mass squared. In order to be able to switch back and forth between both settings we shall view $U''(\varphi) = m(t)^2$ formally as a time dependent mass and carry it along, specifying its origin only when needed. In the field equations $\delta S^\phi/\delta\phi = 0$ a spatial Fourier transform is natural, $\phi(t, x) = \int dp (2\pi)^{-d} e^{ipx} \phi(t, p)$. Then $-\partial_i \delta^{ij} \partial_j$ acts like $p^2 := p_i \delta^{ij} p_i$, which converts the field equation into an ordinary differential equation for each p mode, viz $[(\bar{n}^{-1}\partial_t)^2 + a(t)^{2d} m(t)^2 + a(t)^{2d-2} p^2] \phi(t, p) = 0$.

Homogeneous pure quasifree states:

On a FL background geometry there are, in general, infinitely many physically viable vacuum-like states for a QFT. A vacuum-like state is in particular a "homogeneous pure quasifree" state. A "state" is normally defined algebraically as a positive linear functional over the Weyl algebra [61]. For the present purposes a "state" can be identified with the set of multi-point functions it gives rise to. Then "quasifree" means that all odd n-point functions in the state vanish while the even n-point functions can be expressed in terms of the two-point function $W(t,x;t',x')$ via Wick's theorem. Being a "state" entails certain properties of the two-point function that allow one to realize it via the Gelfand-Naimark-Segal (GNS) construction in the form $(\Omega, u(t,x)u(t',x')\Omega)$, for field operators $u(t,x)$ on vectors Ω in the reconstructed state space. "Pure" means that Ω cannot be written as a convex combination of other states. Finally, for a spatially flat FL background, "homogeneous" just means "translation invariant", i.e. $W(t,x;t',x')$ depends only on $x-x'$.

The GNS reconstructed field operators $u(t,x)$ turn out to coincide with the Heisenberg field operators $\phi(t,x)$ (which are denoted by the same symbol as the classical field, as the latter will no longer occur.) The GNS vector Ω turns out to correspond to a Fock vacuum $|0_T\rangle$, annihilated by annihilation operators defined by a mode expansion of the Heisenberg field operator

$$\begin{aligned}
&\phi(t,x) = \int \frac{dp}{(2\pi)^d} \left[T_p(t)\mathbf{a}_T(p)e^{ipx} + T_p(t)^*\mathbf{a}_T^*(p)e^{-ipx}\right], \\
&\left[\mathbf{a}_T(p), \mathbf{a}_T^*(p')\right] = (2\pi)^d\delta(p-p')\,, \quad \mathbf{a}_T(p)|0_T\rangle = 0\,,
\end{aligned} \tag{190}$$

where $T_p(t)$ is a complex solution of the above classical wave equation, and in the massless case $p = 0$ needs to be excluded in the definition of $|0_T\rangle$. In order for the equal time commutation relations $[\phi(t,p), (\bar{n}^{-1}\partial_t\phi)(t,p')] = i(2\pi)^d\delta(p+p')$ to hold, this solution must obey the Wronskian normalization condition $(\bar{n}^{-1}\partial_t T_p)(t)T_p(t)^* - (\bar{n}^{-1}\partial_t T_p)(t)^* T_p(t) = -i$. Then

$$W(t,x;t',x') = \langle 0_T|\phi(t,x)\phi(t',x')|0_T\rangle = \int \frac{dp}{(2\pi)^d}\, T_p(t)\, T_p(t')^*\, e^{ip(x-x')}\,. \tag{191}$$

One sees that modulo phase choices a "homogeneous pure quasifree" state is characterized

by a choice of Wronskian normalized solution $T_p(t)$ of the wave equation or, equivalently, by a choice of Fock vacuum $|0_T\rangle$ via (190).

Conventions:

We briefly comment on our choice of conventions. In (190) often the $\mathbf{a}_T^*(p)$ is paired with $T_p(t)$ not with $T_p(t)^*$. Then the sign in the Wronskian normalization condition has to be flipped correspondingly. More importantly, we seek to preserve temporal reparameterization invariance by carrying the lapse-like $\bar{n}(t) = \bar{N}(t)/a(t)^d$ along. Since in the wave equation $\bar{n}$ only occurs in the combination $\bar{n}^{-1}\partial_t$, it is convenient to introduce a new time function

$$\tau := \int_{t_i}^{t} dt' \bar{n}(t') \,, \quad \partial_\tau = \bar{n}(t)^{-1}\partial_t \,, \tag{192}$$

for some t_i. Note that $\tau(t) = \tau'(t')$ is a scalar under reparameterizations $t' = \chi^0(t)$ of the coordinate time t, and that $d\tau = dt\bar{n}(t)$, $\bar{n}(t)^{-1}\delta(t,t') = \delta(\tau,\tau')$ are likewise invariant. Here $t' = \chi^0(t)$ with $\chi^0(t_i) = t_i < t_f = \chi^0(t_f)$ must be strictly increasing to qualify as a diffeomorphism. We write $a(\tau)$ for the cosmological scale factor viewed as a function of τ rather than t, and similarly for $m(\tau)$ as well as $T_p(\tau)$. The defining relations for $T_p(\tau)$ then read

$$\begin{aligned} &\big[\partial_\tau^2 + \omega_p(\tau)^2\big] T_p(\tau) = 0 \,, \quad \omega_p(\tau)^2 := a(\tau)^{2d} m(\tau)^2 + p^2 a(\tau)^{2d-2} \,, \\ &\partial_\tau T_p \, T_p^* - \partial_\tau T_p^* \, T_p = -i \,. \end{aligned} \tag{193}$$

This setting has the advantage that the results in different time variables can be obtained by specialization:

$$\begin{aligned} \text{Cosmological time} \;&:\; \bar{n}(t) = a(t)^{-d} \text{ gauge, i.e. } \bar{N}(t) = 1 \,, \\ \text{Conformal time} \;&:\; \bar{n}(t) = a(t)^{1-d} \text{ gauge, i.e. } \bar{N}(t) = a(t) \,, \\ \text{Proper time} \;&:\; \bar{n}(t) = 1 \text{ gauge, i.e. } \bar{N}(t) = a(t)^d \,. \end{aligned} \tag{194}$$

The first two gauges are standard; commonly one writes η for t in conformal time gauge. The last gauge is the FL counterpart of the proper time gauge $\partial_t n(t,x) = 0$ often adopted for the evolution of generic foliated spacetimes.

Generally, $(\bar{n}^{-1}\partial_t)^2 = \bar{n}^{-2}(\partial_t^2 - \bar{n}^{-1}\partial_t\bar{n}\partial_t)$ and the first order term can be removed by the

redefinition $T_p(t) = \bar{n}(t)^{1/2}\chi_p(t)$. This gives

$$\begin{aligned}
&\big[\partial_t^2 + \bar{n}(t)^2\omega_p(t)^2 + \bar{s}(t)\big]\chi_p(t) = 0\,,\\
&\bar{s}(t) := \frac{1}{2}\frac{\partial_t^2\bar{n}}{\bar{n}} - \frac{3}{4}\Big(\frac{\partial_t\bar{n}}{\bar{n}}\Big)^2\,,\\
&\partial_t\chi_p\chi_p^* - (\partial_t\chi_p)^*\chi_p = -i\,.
\end{aligned} \tag{195}$$

In conformal time, $\bar{n}(t) = a(t)^{1-d}$ the coefficient of p^2 is unity and after renaming t into η one has

$$\begin{aligned}
&\Big[\partial_\eta^2 + p^2 + \frac{m(\eta)^2}{a(\eta)^2} + \bar{s}(\eta)\Big]\chi_p(\eta) = 0\,,\\
&\bar{s}(\eta) := -\frac{d-1}{2}\frac{\partial_\eta^2 a}{a} - \frac{(d-3)(d-1)}{4}\Big(\frac{\partial_\eta a}{a}\Big)^2\,,\\
&\partial_\eta\chi_p\chi_p^* - (\partial_\eta\chi_p)^*\chi_p = -i\,.
\end{aligned} \tag{196}$$

We shall occasionally discretize the flat spatial sections of (188), which are isometric to $\mathbb{R}^d$, in order to regularize momentum integrals. A hypercubic lattice $\Lambda = \{x = a_s(n_1,\dots,n_d),\ n_j = 0,\dots,L-1\}$ suffices, with dual lattice $\hat{\Lambda} = \{p = \frac{2\pi}{a_s L}(n_1,\dots,n_d)\,,\ n_j = 0,\dots,L-1\}$, where $a_s > 0$ is the spatial lattice spacing and $L \in \mathbb{N}$ is large. A discretized Fourier transform $\hat{f} : \hat{\Lambda} \to \mathbb{C}$ is defined for real valued functions $f : \Lambda \to \mathbb{R}$ with periodic boundary conditions $f(x + a_s L\hat{\imath}) = f(x)$, $i = 1,\dots,d$. The direct and inverse transforms read

$$\hat{f}(p) = a_s^d \sum_{x\in\Lambda} e^{-ipx} f(x)\,, \quad f(x) = \frac{1}{(a_s L)^d}\sum_{p\in\hat{\Lambda}} e^{ip\cdot x}\hat{f}(p)\,. \tag{197}$$

The continuum limit is taken by first sending $L \to \infty$, which converts $(a_s L)^{-d}\sum_{p\in\hat{\Lambda}}$ into an integral $(2\pi)^{-d}\int d^d p$ over the Brillouin zone $p \in [-\pi/a_s, \pi/a_s]^d$, and then taking $a_s \to 0$. As usual, the lattice Laplacian Δ_s acts by multiplication in Fourier space

$$-\Delta_s\, e^{ip\cdot x} = \hat{p}^2 e^{ip\cdot x}\,, \quad \hat{p}^2 := \sum_{j=1}^d \hat{p}_j^2 = \frac{4}{a_s^2}\sum_{j=1}^d \sin^2\Big(\frac{p_j a_s}{2}\Big)\,. \tag{198}$$

Unless confusing we shall set $a_s = 1$ and omit the 'hat' on the Fourier transformed functions.

Heisenberg picture:

Time evolution in the Heisenberg picture is generated by the canonical Hamiltonian

derived from (189) with the field operators (190) inserted. After Fourier decomposition this leads to

$$\begin{aligned}
\mathbb{H}(\tau) &= \int \frac{dp}{(2\pi)^d}\, \mathbb{H}_p(\tau)\,, \qquad \omega_p(\tau)^2 := m(\tau)^2 a(\tau)^{2d} + p^2 a(\tau)^{2d-2}\,, \\
\mathbb{H}_p(\tau) &= \frac{1}{2}|\pi(\tau,p)|^2 + \frac{1}{2}\omega_p(\tau)^2 |\phi(\tau,p)|^2 \qquad (199)\\
&= \frac{1}{2}\big(|\partial_\tau T_p|^2 + \omega_p(\tau)^2 |T_p|^2\big)\big(\mathbf{a}_T(-p)\mathbf{a}_T^*(-p) + \mathbf{a}_T^*(p)\mathbf{a}_T(p)\big) \\
&+ \frac{1}{2}\big((\partial_\tau T_p)^2 + \omega_p(\tau)^2 T_p^2\big)\mathbf{a}_T(-p)\mathbf{a}_T(p) + \frac{1}{2}\big((\partial_\tau T_p^*)^2 + \omega_p(\tau)^2 (T_p^*)^2\big)\mathbf{a}_T^*(p)\mathbf{a}_T^*(-p)\,.
\end{aligned}$$

In particular

$$\begin{aligned}
\partial_\tau \phi(\tau,p) &= i[\mathbb{H}(\tau), \phi(\tau,p)] = \pi(\tau,p)\,, \\
\partial_\tau \pi(\tau,p) &= i[\mathbb{H}(\tau), \pi(\tau,p)] = -\omega_p(\tau)^2 \phi(\tau,p)\,, \qquad (200)
\end{aligned}$$

are the Heisenberg picture evolution equations. For later use we prepare their solution in terms of the (real, anti-symmetric) commutator function $\Delta_p(\tau',\tau)$ defined by

$$\begin{aligned}
&\big[\partial_\tau^2 + \omega_p(\tau)^2\big]\Delta_p(\tau,\tau_0) = 0 = \big[\partial_{\tau_0}^2 + \omega_p(\tau_0)^2\big]\Delta_p(\tau,\tau_0)\,, \\
&\Delta_p(\tau,\tau_0) = -\Delta_p(\tau_0,\tau)\,, \quad \partial_\tau \Delta_p(\tau,\tau_0)\big|_{\tau=\tau_0} = 1\,. \qquad (201)
\end{aligned}$$

The terminology of course refers to the relations

$$\begin{aligned}
i[\phi(\tau,p), \phi(\tau_0,p_0)] &= (2\pi)^d \delta(p+p_0)\Delta_p(\tau,\tau_0)\,, \\
\Delta_p(\tau,\tau_0) &:= i\big(T_p(\tau)T_p(\tau_0)^* - T_p(\tau)^* T_p(\tau_0)\big)\,, \qquad (202)
\end{aligned}$$

so that $\partial_\tau \Delta_p(\tau,\tau_0)|_{\tau=\tau_0} = 1$ codes the equal time commutation relations. Note that any other Wronskian normalized complex solution defines the same commutator function, see Lemma 5.2.3. The solution of the evolution equations (200) then reads

$$\begin{aligned}
\phi(\tau,p) &= \Delta_p(\tau,\tau_0)\pi(\tau_0,p) - \partial_{\tau_0}\Delta_p(\tau,\tau_0)\phi(\tau_0,p)\,, \\
\pi(\tau,p) &= \partial_\tau\Delta_p(\tau,\tau_0)\pi(\tau_0,p) - \partial_\tau\partial_{\tau_0}\Delta_p(\tau,\tau_0)\phi(\tau_0,p)\,. \qquad (203)
\end{aligned}$$

The central object later on will be the Hamilton operator (199) averaged with a smooth positive window function $f(\tau)^2$ of compact support in (τ_i, τ_f). This may be normalized so that $\int d\tau f(\tau)^2 = 1$. We write

$$\begin{aligned}\int d\tau f(\tau)^2\, \mathbb{H}_p(\tau) &= \mathcal{E}_p[T]\big(\mathbf{a}_T(-p)\mathbf{a}_T^*(-p) + \mathbf{a}_T^*(p)\mathbf{a}_T(p)\big) \\ &+ \mathcal{D}_p[T]\, \mathbf{a}_T(-p)\mathbf{a}_T(p) + \mathcal{D}_p[T]^*\, \mathbf{a}_T^*(p)\mathbf{a}_T^*(-p)\,, \end{aligned} \tag{204}$$

with

$$\begin{aligned}\mathcal{E}_p[T] &:= \frac{1}{2}\int d\tau\, f(\tau)^2 \left\{|\partial_\tau T_p|^2 + \omega_p(\tau)^2 |T_p|^2\right\} > |\mathcal{D}_p[T]|\,, \\ \mathcal{D}_p[T] &:= \frac{1}{2}\int d\tau f(\tau)^2 \left\{(\partial_\tau T_p)^2 + \omega_p(\tau)^2 T_p^2\right\}. \end{aligned} \tag{205}$$

The above formulation preserves temporal reparameterization invariance through the use of τ from (192). As a consequence, the solutions of the wave equation (193) can be interpreted as functions of the coordinate time t with a functional dependence on $\bar{n}$. We shall occasionally do so and then (by slight abuse of notation) keep the function symbols, writing $T_p(\tau) = T_p(t)$, etc.. When fixing a gauge as in (194) one will however normally absorb additional powers of $a(t)$ into a redefined averaging function and frequency. Specifically,

$$\mathcal{E}_p[T] = \frac{1}{2}\int dt\, f(t)^2 \bar{n}(t)^{-1} \left\{|\partial_t T_p|^2 + (\bar{n}(t)\omega_p(t))^2 |T_p|^2\right\}, \tag{206}$$

motivates

$$\begin{aligned} f^{\mathrm{cosm}}(t)^2 &:= f(t)^2 a(t)^d\,, & \omega_p^{\mathrm{cosm}}(t) &:= a(t)^{-d}\omega_p(t)\,, \\ f^{\mathrm{conf}}(t)^2 &:= f(t)^2 a(t)^{d-1}\,, & \omega_p^{\mathrm{conf}}(t) &:= a(t)^{1-d}\omega_p(t)\,, \\ f^{\mathrm{prop}}(t)^2 &:= f(t)^2\,, & \omega_p^{\mathrm{prop}}(t) &:= \omega_p(t)\,. \end{aligned} \tag{207}$$

In cosmological time gauge this matches the conventions in [80].

The functional $\mathcal{E}_p[T]$ can be related to a point-split subtracted version of the 00-component of the energy momentum tensor [80, 45] and as such can be interpreted as the energy *density* of a given p mode. The same interpretation arises when the spatial sections are discretized. In the conventions of (197), the main change is that the commutation relations in (190) are

replaced by $[\mathbf{a}_T(p), \mathbf{a}_T^*(p')] = L^d \delta_{p,p'}$. This gives $\mathcal{E}_p[T]$ (without subtractions) the interpretation as the energy density of the Hamiltonian's temporal average. Indeed, from (204) one has

$$\langle 0_T | \int d\tau f(\tau)^2 \mathbb{H}_p(\tau) | 0_T \rangle = L^d \mathcal{E}_p[T] \,. \tag{208}$$

Schrödinger picture:

Recall that the Heisenberg picture and the Schrödinger picture are related by a unitary transformation implemented by the propagation operator $U(\tau, \tau_0)$. The Schrödinger picture is designed such that expectation values are the same as in the Heisenberg picture but the dynamical evolution is attributed to the states. Whence

$$|\psi; \tau\rangle_{\mathsf{s}} := U(\tau, \tau_0)^{-1} |\psi\rangle \,, \quad A_{\mathsf{s}}(\tau) := U(\tau, \tau_0)^{-1} A(\tau) U(\tau, \tau_0) \,. \tag{209}$$

Here $A(\tau)$ carries both the dynamical and potentially an explicit time dependence while $A_{\mathsf{s}}(\tau)$ carries only the residual explicit time dependence. The states $|\psi\rangle$ are normalizable and time independent while the Schrödinger picture states evolve according to

$$i\partial_\tau |\psi; \tau\rangle_{\mathsf{s}} = \mathbb{H}_{\mathsf{s}}(\tau) |\psi; \tau\rangle_{\mathsf{s}} \,, \quad \mathbb{H}_{\mathsf{s}}(\tau) := U(\tau, \tau_0)^{-1} \mathbb{H}(\tau) U(\tau, \tau_0) \,. \tag{210}$$

This is such that $\langle \psi | A(\tau) | \psi \rangle = {}_{\mathsf{s}}\langle \psi; \tau | A_{\mathsf{s}}(\tau) | \psi; \tau \rangle_{\mathsf{s}}$. As the propagation operator's generator one can alternatively take $\mathbb{H}(\tau)$ or $\mathbb{H}_{\mathsf{s}}(\tau)$; in terms of the path ordered exponentials one formally has

$$U(\tau, \tau_0) = \exp_+ \left\{ i \int_{\tau_0}^{\tau} ds \, \mathbb{H}(s) \right\} = \exp_- \left\{ i \int_{\tau_0}^{\tau} ds \, \mathbb{H}_{\mathsf{s}}(s) \right\} , \tag{211}$$

where $\exp_+$ orders the operators from left to right in decreasing order of the argument and vice versa for $\exp_-$. Similar relations exist for the inverse. Note that only the $\exp_+$ versions will satisfy the usual composition law. Results on convergence properties will not be needed.

For the basic operators of our scalar QFT the Schrödinger picture operators can be identified with the initial values of the Heisenberg picture operators. We transition to a lattice description (in order for the Schrödinger picture to be rigorously defined) with $a_s = 1$

and write

$$\phi_{\mathsf{s}}(p) = \phi(\tau_0, p) =: u(p)\,, \quad \pi_{\mathsf{s}}(p) = \pi(\tau_0, p) =: -iL^d \frac{\delta}{\delta u(-p)}\,, \quad p \in \hat{\Lambda}\,. \tag{212}$$

For the Hamiltonian this gives

$$\mathbb{H}_{\mathsf{s}}(\tau) = \frac{1}{2L^d} \sum_{p\in\hat{\Lambda}} \Big\{ - L^{2d} \frac{\delta^2}{\delta u(p)\delta u(-p)} + \omega_p(\tau)^2 u(p)u(-p) \Big\}\,. \tag{213}$$

The matrix elements of the time averaged Heisenberg picture Hamiltonian become the time averages of the Schrödinger picture matrix elements

$$\begin{aligned} \langle\psi| \int d\tau f(\tau)^2\, \mathbb{H}(\tau)|\psi\rangle &= \int d\tau\, f(\tau)^2 {}_{\mathsf{s}}\langle\psi;\tau|\mathbb{H}_{\mathsf{s}}(\tau)|\psi;\tau\rangle_{\mathsf{s}} \\ &= \int d\tau\, f(\tau)^2 {}_{\mathsf{s}}\langle\psi;\tau|i\partial_\tau|\psi;\tau\rangle_{\mathsf{s}}\,. \end{aligned} \tag{214}$$

We state without derivation the counterpart of the Fock vacuum $|0_T\rangle$ in the Schrödinger picture, see [44, 65, 66, 62] for related accounts.

Proposition 5.2.1. The Schrödinger picture state $|\Omega_T;\tau\rangle_{\mathsf{s}} := U(\tau,\tau_0)^{-1}|0_T\rangle$ evaluates on a finite lattice Λ to

$$\begin{aligned} \Omega_T[u] &= \mathcal{N}(\tau) \exp\Big\{ \frac{i}{2L^d} \sum_{p\in\hat{\Lambda}} \Xi_p(\tau) u(p)u(-p) \Big\}\,. \\ \Xi_p(\tau) &= \frac{\partial_\tau T_p(\tau)^*}{T_p(\tau)^*} = \frac{i + \partial_\tau |T_p(\tau)|^2}{2|T_p(\tau)|^2}\,, \end{aligned} \tag{215}$$

with $\mathcal{N}(\tau) = \Omega_T[0]$. Separating modulus and phase, $\Omega_T[u] = |\Omega_T[u]|e^{iA_T[u]}$, one has

$$\begin{aligned} |\Omega_T[u]| &= |\Omega_0(\tau)| \prod_{p\neq 0} |\Omega_p(\tau)|\,, \quad A_T[u] = A_0(\tau) + \sum_{p\neq 0} A_p(\tau) \\ |\Omega_0(\tau)| &= \frac{1}{(2\pi L^d)^{1/4}} \frac{1}{\sqrt{T_0(\tau)}} \exp\Big\{ - \frac{u_0^2}{4L^d|T_0(\tau)|^2} \Big\}\,, \\ |\Omega_p(\tau)| &= \frac{1}{(\pi L^d)^{1/4}} \frac{1}{\sqrt{T_p(\tau)}} \exp\Big\{ - \frac{u_p^2}{4L^d|T_p(\tau)|^2} \Big\}\,, \\ A_0(\tau) &= \frac{1}{2} \arg T_0(\tau) + \frac{1}{2L^d} \partial_\tau \ln |T_0(\tau)| u_0^2\,, \\ A_p(\tau) &= \frac{1}{2} \arg T_p(\tau) + \frac{1}{2L^d} \partial_\tau \ln |T_p(\tau)|\, |u_p|^2\,, \end{aligned} \tag{216}$$

with normalization

$$\int \prod_p du(p) |\Omega_T[u]|^2 := \int du_0 |\Omega_0(\tau)|^2 \int \prod_{p_d>0} du(p) |\Omega_p(\tau)|^4 = 1\,. \tag{217}$$

With this in place we can return to (214) and evaluate

$${}_{\mathsf{s}}\langle \Omega_T;\tau | i\partial_\tau | \Omega_T;\tau\rangle_{\mathsf{s}} = \int \prod_p du(p) \Big\{ \frac{i}{2} \partial_\tau |\Omega_T[u]|^2 - \partial_\tau A_T[u] |\Omega_T[u]|^2 \Big\}\,. \tag{218}$$

The imaginary part vanishes because $\Omega_T[u]$ is L^2 normalized. The real part essentially is a Gaussian with a $|u|^2$ insertion. We interpret $|\Omega[u]|$ as in (216) and find

$${}_{\mathsf{s}}\langle \Omega_T;\tau | i\partial_\tau | \Omega_T;\tau\rangle_{\mathsf{s}} \;=\; -\frac{1}{2} \sum_p \Big\{ |T_p(\tau)|^2 \partial_\tau^2 \ln |T_p(\tau)| + \partial_\tau \arg T_p(\tau) \Big\}\,. \tag{219}$$

Next we use

$$\partial_\tau \arg T_p(\tau) = \frac{1}{2i} \partial_\tau \ln \frac{T_p(\tau)}{T_p(\tau)^*} = -\frac{1}{2|T_p(\tau)|^2}\,, \quad \partial_\tau^2 \xi_p + \omega_p(\tau)^2 \xi_p = \frac{1}{4\xi_p^3}\,, \tag{220}$$

with $\xi_p(\tau) := |T_p(\tau)|$. The differential equation for ξ_p is the Ermakov-Pinney equation. Together

$$\begin{aligned} {}_{\mathsf{s}}\langle \Omega_T;\tau | i\partial_\tau | \Omega_T;\tau\rangle_{\mathsf{s}} \;&=\; \frac{1}{2} \sum_p \Big\{ (\partial_\tau \xi_p)^2 + \omega_p(\tau)^2 \xi_p^2 + \frac{1}{4\xi_p^2} \Big\} \\ &=\; \frac{1}{2} \sum_p \Big\{ |\partial_\tau T_p(\tau)|^2 + \omega_p(\tau)^2 |T_p(\tau)|^2 \Big\}\,. \end{aligned} \tag{221}$$

Upon temporal averaging the right hand side equals $\sum_p \mathcal{E}_p[T]$, with $\mathcal{E}_p[T]$ from (205). Hence

$$\int d\tau\, f(\tau)^2\, {}_{\mathsf{s}}\langle \Omega_T;\tau | i\partial_\tau | \Omega_T;\tau\rangle_{\mathsf{s}} = \sum_p \mathcal{E}_p[T]\,. \tag{222}$$

As expected, the right hand side equals the $L^{-d} \sum_p$ summation over p-fibres of (208) in the Heisenberg picture. The Schrödinger picture, however, lends itself to a different minimization procedure described in Section 5.2.3.

5.2.2 SLE in Heisenberg picture and independence of fiducial states

So far T_p has been an arbitrary solution of (193). We now regard $\mathcal{E}_p[T]$ from (205) as a functional of T_p and aim at minimizing it for fixed p. This is a finite dimensional minimization problem because the solutions of (205) are in one-to-one correspondence to their Wronskian normalized complex initial data. We shall pursue this route towards minimization in Section 5.2.3.

SLE via fiducial solutions:

Alternatively, one can fix a fiducial solution $S_p(\tau)$ of (193) and write any solution in the form

$$T_p(\tau) = \lambda_p S_p(\tau) + \mu_p S_p(\tau)^* \,, \quad |\lambda_p|^2 - |\mu_p|^2 = 1 \,. \tag{223}$$

With S_p and p held fixed the minimization is then over the parameters $\lambda_p, \mu_p \in \mathbb{C}$. Since $e^{-i\mathrm{Arg}\mu_p} T_p(\tau)$ is a solution of (193) if $T_p(\tau)$ is we may assume without loss of generality that μ_p is real. Since $|\lambda_p| = \sqrt{1+\mu_p^2}$, only μ_p and the phase of λ_p are real parameters over which the minimum of $\mathcal{E}_p[T_p]$ is sought. Inserting (223) with the simplified parameterization into (205) one has

$$\begin{aligned} \mathcal{E}_p[T] &= (1+2\mu_p^2)\mathcal{E}_p[S] + \mu_p\sqrt{1+\mu_p^2}\big(e^{i\arg\lambda_p}\mathcal{D}_p[S] + e^{-i\arg\lambda_p}\mathcal{D}_p[S]^*\big) \,, \\ \mathcal{D}_p[T] &= (1+\mu_p^2)e^{2i\arg\lambda_p}\mathcal{D}_p[S] + \mu_p^2\mathcal{D}_p[S]^* + 2\mu_p\sqrt{1+\mu_p^2}e^{i\arg\lambda_p}\mathcal{E}_p[S] \,. \end{aligned} \tag{224}$$

Clearly, the minimizing phase is such that $e^{i\arg\lambda_p}e^{i\arg\mathcal{D}_p[S]} = -1$. The minimization in μ_p then is straightforward and results in [80]

$$\mu_p = \sqrt{\frac{c_1}{2\sqrt{c_1^2-|c_2|^2}} - \frac{1}{2}} \,, \quad \lambda_p = -\,e^{-i\,\mathrm{Arg}\,c_2}\sqrt{\frac{c_1}{2\sqrt{c_1^2-|c_2|^2}} + \frac{1}{2}} \,, \tag{225}$$

where whenever the fixed fiducial solution is clear from the context one sets

$$\begin{aligned} c_1 &:= \mathcal{E}_p[S] = \frac{1}{2}\int d\tau f(\tau)^2\big[|\partial_\tau S_p|^2 + \omega_p^2|S_p|^2\big] > |c_2| \,, \\ c_2 &:= \mathcal{D}_p[S] = \frac{1}{2}\int d\tau f(\tau)^2\big[(\partial_\tau S_p)^2 + \omega_p^2 S_p^2\big] \,. \end{aligned} \tag{226}$$

Since only a phase choice has been made in arriving at (226) it is clear that the minimizing

linear combination is unique up to a phase, *for a fixed fiducial solution* S. It is called the *State of Low Energy* (SLE) solution of (193) with fiducial solution S. We write

$$T_{S,p}(\tau) := \lambda_p[S]S_p[\tau] + \mu_p[S]S_p(\tau)^*\,, \tag{227}$$

with $\lambda_p[S], \mu_p[S]$ the functionals from (225), (226). Olbermann's theorem [80] states that the homogeneous pure quasifree state associated with $T_S(\tau)$ via (191) is an *exact* Hadamard state. This is an important result which improves earlier ones based on the adiabatic expansion in several ways, as noted in the introduction. Its practical usefulness is somewhat hampered by the fact that one still needs to know an exact solution S of the wave equation to begin with and that the resulting Hadamard state off-hand depends on the choice of S. The second caveat is addressed in Theorem 5.2.1 below. In preparation, we note the following proposition, where we omit the subscript p for simplicity.

Proposition 5.2.2. Consider the following functionals: $\mathcal{I} : C[\tau_i, \tau_f] \to \mathbb{R}_+ \cup \{0\}$, and $\mathcal{J}, \mathcal{K} : C[\tau_i, \tau_f] \to C[\tau_i, \tau_f]$

$$\begin{aligned}
\mathcal{I}[S] &:= \mathcal{E}[S]^2 - |\mathcal{D}[S]|^2\,,\\
\mathcal{J}[S](\tau) &:= 2\mathcal{E}[S]|S(\tau)|^2 - \mathcal{D}[S]^* S(\tau)^2 - \mathcal{D}[S]S(\tau)^{*2}\,,\\
\mathcal{K}[S](\tau) &:= 2\mathcal{E}[S]|\partial_\tau S(\tau)|^2 - \mathcal{D}[S]^*[\partial_\tau S(\tau)]^2 - \mathcal{D}[S][\partial_\tau S(\tau)^*]^2\,.
\end{aligned} \tag{228}$$

For $a, b \in \mathbb{C}$ they obey

$$\begin{aligned}
\mathcal{I}[aS + bS^*] &= (|a|^2 - |b|^2)^2\,\mathcal{I}[S]\,,\\
\mathcal{J}[aS + bS^*](\tau) &= (|a|^2 - |b|^2)^2\,\mathcal{J}[S](\tau)\,,\\
\mathcal{K}[aS + bS^*](\tau) &= (|a|^2 - |b|^2)^2\,\mathcal{K}[S](\tau)\,.
\end{aligned} \tag{229}$$

This may be proven by lengthy direct computations; we shall present a more elegant derivation based on properties of the commutator function in Section 5.2.3.

Theorem 5.2.1.

(a) The SLE two-point function based on a fiducial solution S

$$W[S](\tau, x; \tau', x') := \int \frac{d^d p}{(2\pi)^d} e^{ip(x-x')} T_{S,p}(\tau) T_{S,p}(\tau')^* \,, \tag{230}$$

is a Bogoliubov invariant, i.e. $W[aS + bS^*] = W[S]$, with $a, b \in \mathbb{C}$, $|a|^2 - |b|^2 = 1$. Hence $W[S]$ is independent of the choice of the fiducial solution S.

(b) The modulus of an SLE solution can be written as a ratio of Bogoliubov invariants from Proposition 5.2.2.

$$|T_{S,p}(\tau)|^2 = \frac{\mathcal{J}_p[S](\tau)}{2\sqrt{\mathcal{I}_p[S]}} \,. \tag{231}$$

This also implies (a).

Proof.

For readability's sake, we omit the subscript p in the following.

(a) We first show that a minimum T of $\mathcal{E}$ is a zero of $\mathcal{D}$. Assume to the contrary that T minimizes $\mathcal{E}$ but $\mathcal{D}[T] \neq 0$. Consider $\mu T + \lambda T^*$, with $\mu > 0, \lambda = e^{i \arg \lambda}\sqrt{1+\mu^2}$ and compute $\mathcal{E}[\mu T + \lambda T^*]$ as in (224)

$$\mathcal{E}[\mu T + \lambda T^*] = (1 + 2\mu^2)\mathcal{E}[T] + 2\mu \Re\big(\lambda \mathcal{D}[T]\big) \,. \tag{232}$$

Then there exists a $\mu \neq 0$ such that $\mathcal{E}[\mu T + \lambda T^*] < \mathcal{E}[T]$, contradicting the assumption that T minimizes $\mathcal{E}$. Subject to the minimizing phase choice $e^{-i \arg \lambda} e^{i \arg \mathcal{D}[S]} = -1$ one can also see from (224) that $(\partial \mathcal{E}[T]/\partial \mu)$ is proportional to $\mathcal{D}[T]$.

Let now T_{S_1}, T_{S_2} be two minimizers of $\mathcal{E}$ associated with fiducial solutions S_1, S_2. Then there exist some a, $b \in \mathbb{C}$ with $|a|^2 - |b|^2 = 1$ such that $T_{S_2} = aT_{S_1} + bT_{S_1}^*$. Further, $e^{-i \arg b} T_{S_2}$ is of the form used in (232) so that

$$\mathcal{E}[e^{-i \arg b} T_{S_2}] = \mathcal{E}[T_{S_2}] = (2b^2 + 1)\, \mathcal{E}[T_{S_1}] + 2b\, \Re[a\, \mathcal{D}(T_{S_1})] \,. \tag{233}$$

By the previous step, $\mathcal{D}(T_{S_1}) = 0$ as T_{S_1} is a minimizer of $\mathcal{E}$. Therefore (233) reduces to $\mathcal{E}[T_{S_2}] = (2b^2+1)\, \mathcal{E}[T_{S_2}]$. Since $\mathcal{E}[T_{S_2}] = \mathcal{E}[T_{S_1}]$ we must have $b = 0$. Hence $e^{-i \arg b} T_{S_2} = T_{S_1}$, which implies (a).

(b) The expression (231) follows by direct computation. Hence (229) implies (a) via

$|T_{S_1}(\tau)| = |T_{S_2}(\tau)|$, as any two fiducial solutions S_1, S_2 must be related by $S_2 = aS_1 + bS_2^*$, $|a|^2 - |b|^2 = 1$. This also implies (a) since a Wronskian normalized solution of (193) is uniquely determined by its modulus, up to a time independent (but potentially p dependent) phase. □

Remarks:

(i) Uniqueness up a phase of the SLE modes has been asserted in Theorem 3.1 of [80] and justified (in the line preceding it) by noting that only a phase choice is being made in the process of obtaining the solution formulas (225). In itself, however, this only yields uniqueness *relative* to a choice of fiducial solution, as indicated in (227). We are not aware of a presentation of SLE [80, 45, 28, 96] alluding to results of the above type. Lemma 4.5 of [80] shows the independence of a SLE solution from the order of the adiabatic vacuum used as a fiducial solution. This, however, only concerns the large momentum behavior, while Theorem 5.2.1 ascertains the independence (up to a phase) from *any* fiducial solution at *all* momenta.

(ii) Writing momentarily $\mathcal{E}_S(\mu, \arg\lambda)$ for the right hand side of $\mathcal{E}[T]$ in (224) one can of course trade a Bogoliubov transformation in S for one in the parameters. This gives $\mathcal{E}_{S_1}(\mu_1, \arg\lambda_1) = \mathcal{E}_{S_2}(\mu_2, \arg\lambda_2)$ for any two fiducial solutions. For this to imply the existence of a unique minimum the gradients of $\mathcal{E}_{S_1}$ and $\mathcal{E}_{S_2}$ must be related by a 2×2 matrix which remains nonsingular on a zero of one (and then both) gradient(s). Further, the Hessian must be positive definite on a zero of the gradient. The above proof validates these properties, but they are not consequences merely of the fact that (225) is unique up to a choice of phase.

(iii) By rewriting (224) in matrix form one finds the minimizing parameters (225) to diagonalize the original $c_1 = \mathcal{E}[S], c_2 = \mathcal{D}[S]$ matrix

$$\begin{pmatrix} \mathcal{E}[T_S] & \mathcal{D}[T_S] \\ \mathcal{D}[T_S]^* & \mathcal{E}[T_S] \end{pmatrix} = \begin{pmatrix} \lambda & \mu \\ \mu & \lambda^* \end{pmatrix} \begin{pmatrix} c_1 & c_2 \\ c_2^* & c_1 \end{pmatrix} \begin{pmatrix} \lambda^* & \mu \\ \mu & \lambda \end{pmatrix} = \begin{pmatrix} \sqrt{c_1^2 - |c_2|^2} & 0 \\ 0 & \sqrt{c_1^2 - |c_2|^2} \end{pmatrix} . \tag{234}$$

The off-diagonal entries confirm the "Minimizer of $\mathcal{E}$ is a zero of $\mathcal{D}$" assertion in part (a) of the proof of Theorem 5.2.1; the diagonal entries display the value of the minimizing energy $\mathcal{E}[T_S]$. In fact, the relation (234) could be taken as an alternative definition of the coefficients

λ, μ with solution (225).

Minimization in Fock space:

We temporarily return to the lattice formulation. The minimization of $\mathcal{E}_p[T]$ already assumed that the time averaged Hamiltonian $\int d\tau f(\tau)^2 \mathbb{H}_p(\tau)$ is evaluated in the coordinated Fock vacuum $|0_T\rangle$, see (208). The operator (204) itself has well-defined expectation values on a dense subspace $\mathcal{F}_0$ of the Fock space on which it is also selfadjoint and positive semidefinite. Hence

$$\inf_{\psi \in \mathcal{F}_0} \frac{\langle \psi | \int d\tau \, f(\tau)^2 \, \mathbb{H}_p(\tau) | \psi \rangle}{\langle \psi | \psi \rangle} = E_p^{\inf} \,, \tag{235}$$

is well defined with some $E_p^{\inf} \geq 0$. By the min-max theorem for (possibly unbounded) selfadjoint operators [88], the quantity $E_p^{\inf}$ also coincides with the infimum of the spectrum of $\int d\tau \, f(\tau)^2 \, \mathbb{H}_p(\tau)$. In order to determine the infimum of the spectrum one can try to diagonalize the operator. Using (204), (234), one has

$$\begin{aligned} \int d\tau f(\tau)^2 \, \mathbb{H}_p(\tau) &= \big(\mathbf{a}_S(-p), \mathbf{a}_S^*(p)\big) \begin{pmatrix} \mathcal{E}_p[S] & \mathcal{D}_p[S] \\ \mathcal{D}_p[S]^* & \mathcal{E}_p[S] \end{pmatrix} \begin{pmatrix} \mathbf{a}_S^*(-p) \\ \mathbf{a}_S(p) \end{pmatrix} \\ &= \mathcal{E}_p[T_S] \big(\mathbf{a}_{T_S}(-p) \mathbf{a}_{T_S}^*(-p) + \mathbf{a}_{T_S}^*(p) \mathbf{a}_{T_S}(p) \big) \,. \end{aligned} \tag{236}$$

From (236) it is clear that the infimum of the spectrum is a minimum and is assumed if $|\psi\rangle = |0_{T_S}\rangle$ is the Fock vacuum associated with the SLE solution. Hence

$$E_p^{\inf} = \mathcal{E}_p[T_S] = \sqrt{\mathcal{E}_p[S]^2 - |\mathcal{D}_p[S]|^2} \,. \tag{237}$$

Since the operator in (235) can be written in an arbitrary Bogoliubov frame one would expect that the infimum is a Bogoliubov invariant. By Proposition 5.2.2 this indeed the case.

Instantaneous limit:

In general, the Fock vacuum $\mathbf{a}_T(p)|0_T\rangle = 0$ is not an eigenstate of $\mathbb{H}_p(\tau)$. At any fixed time τ_0 one has however:

$$\begin{aligned} & |\partial_\tau T_p(\tau_0)|^2 + \omega_p(\tau_0)^2 |T_p(\tau_0)|^2 \stackrel{!}{=} \min \,, \\ \text{iff} \quad & T_p(\tau_0) = \frac{e^{i\nu_0}}{\sqrt{2\omega_p(\tau_0)}} \,, \quad (\partial_\tau T_p)(\tau_0) = -ie^{i\nu_0} \sqrt{\frac{\omega_p(\tau_0)}{2}} \,. \\ \text{iff} \quad & [\partial_\tau T_p(\tau_0)]^2 + \omega_p(\tau_0)^2 T_p(\tau_0)^2 = 0 \,, \end{aligned} \tag{238}$$

for some $\nu_0 \in [0, 2\pi)$. Note that in Minkowski space the minimization reproduces $T_p(t) = e^{-it\omega_p}/\sqrt{2\omega_p}$, $\omega_p = \sqrt{p^2 + m_0^2}$. Generally, the value of the minimum in the first line is $\omega_p(\tau_0)$. With the choice (238) of minimizing mode 'functions' the Hamilton operator *at* τ_0 simplifies to

$$\mathbb{H}(\tau_0) = \frac{1}{2}\int \frac{dp}{(2\pi)^d}\omega_p(\tau_0)\big(\mathbf{a}_{\tau_0}(p)\mathbf{a}^*_{\tau_0}(p) + \mathbf{a}^*_{\tau_0}(p)\mathbf{a}_{\tau_0}(p)\big)\,. \tag{239}$$

On a finite lattice this also turns the Fock vacuum $\mathbf{a}_{\tau_0}(p)|0_{\tau_0}\rangle = 0$ into the ground state of $\mathbb{H}(\tau_0)$. This "instantaneous diagonalization" has originally been pursued in an attempt to introduce a particle concept at each instant. The "instantaneous Fock vacuum" $|0_{\tau_0}\rangle$ does however *not* give rise to a physically viable state, as for $\tau \neq \tau_0$ the norm-squared of the normal-ordered Hamiltonian, $\langle 0_{\tau_0}| : \mathbb{H}(\tau) :: \mathbb{H}(\tau) : |0_{\tau_0}\rangle$, in general diverges [41, 36]. The temporal averaging resolves this problem in a simple and satisfactory manner.

Consistency requires that in the instantaneous limit $f(\tau)^2 \to \delta(\tau - \tau_0)$ the SLE solution (227) reduces to the one in (238). One can check that this indeed the case

$$\begin{aligned} T_{S,p}(\tau_0) = \lambda_p[S]S_p(\tau_0) + \mu_p[S]S^*_p(\tau_0) \quad &\longrightarrow \quad \frac{1}{\sqrt{2\omega_p(\tau_0)}}\,, \\ \partial_\tau T_{S,p}(\tau_0) = \lambda_p[S](\partial_\tau S_p)(\tau_0) + \mu_p[S](\partial_\tau S_p)^*(\tau_0) \quad &\longrightarrow \quad -i\sqrt{\frac{\omega_p(\tau_0)}{2}}\,. \end{aligned} \tag{240}$$

5.2.3 SLE in Schrödinger picture and minimization over initial data

As seen in (235), (237) a SLE can be obtained by a minimization over the state space in the Heisenberg picture. The relevant matrix element can be transcribed into the Schrödinger picture via (214). Since the state vectors now evolve, the natural minimization is over their initial vectors $|\psi; \tau_0\rangle_S$, which can be identified with the Heisenberg picture states. The minimization in the Schrödinger picture therefore assumes the form

$$\inf_{|\psi;\tau_0\rangle_{\mathsf{s}} \in \mathcal{F}_0} \int d\tau\, f(\tau)^2\, {}_{\mathsf{s}}\langle\psi;\tau|i\partial_\tau|\psi;\tau\rangle_{\mathsf{s}}\,. \tag{241}$$

The Fock vacua correspond to time dependent Gaussians (215), (216) satisfying the functional Schrödinger equation. The identity (222) shows that the functional $\mathcal{E}_p$ on the space of solutions of the wave equation to be minimized is the same as in the Heisenberg picture.

However, the relevant parameters are now the *initial data*.

In order to reformulate the minimization problem as one with respect to the initial data we proceed as follows. The solution formula (203) can be applied to the mode functions themselves giving

$$T_p(\tau) = \Delta_p(\tau,\tau_0)\partial_{\tau_0}T_p(\tau_0) - \partial_{\tau_0}\Delta_p(\tau,\tau_0)T_p(\tau_0)\,. \tag{242}$$

Inserting (242) and its time derivative into the definitions of $\mathcal{E}_p$ and $\mathcal{D}_p$ gives

$$\begin{aligned}\mathcal{E}_p &= J_p(\tau_0)|w_p|^2 + K_p(\tau_0)|z_p|^2 - \partial_{\tau_0}J_p(\tau_0)\Re(w_pz_p)\,,\\ \mathcal{D}_p &= J_p(\tau_0)w_p^2 + K_p(\tau_0)z_p^2 - \partial_{\tau_0}J_p(\tau_0)w_pz_p\,,\end{aligned} \tag{243}$$

with $z_p := T_p(\tau_0)$, $w_p := \partial_{\tau_0}T_p(\tau_0)$, subject to $w_pz_p^* - w_p^*z_p = -i$. The coefficients

$$\begin{aligned}J_p(\tau_0) &= \frac{1}{2}\int d\tau\, f(\tau)^2\big[\big(\partial_\tau\Delta_p(\tau,\tau_0)\big)^2 + \omega_p(\tau)^2\Delta_p(\tau,\tau_0)^2\big]\,,\\ K_p(\tau_0) &= \frac{1}{2}\int d\tau\, f(\tau)^2\big[\big(\partial_\tau\partial_{\tau_0}\Delta_p(\tau,\tau_0)\big)^2 + \omega_p(\tau)^2\big(\partial_{\tau_0}\Delta_p(\tau,\tau_0)\big)^2\big]\,,\end{aligned} \tag{244}$$

are manifestly positive and are invariant under Bogoliubov transformations because the commutator function is. They are also independent of the initial data because $\Delta_p(\tau,\tau_0)$ is uniquely characterized by (201). No reference to any fiducial solution is made, instead $\mathcal{E}_p, \mathcal{D}_p$ in (243) are functions of the constrained complex initial data z_p, w_p.

Neither the sign nor the modulus of of $\partial_{\tau_0}J_p(\tau_0)$ is immediate. For the subsequent analysis we anticipate the inequality

$$4K_p(\tau_0)J_p(\tau_0) - (\partial_{\tau_0}J_p(\tau_0))^2 > 0\,. \tag{245}$$

Further we momentarily simplify the notation by writing $K, J, \dot{J}$ for $K_p(\tau_0), J_p(\tau_0), \partial_{\tau_0}J_p(\tau_0)$, respectively. In addition we omit the subscripts p from $z_p, w_p, \mathcal{E}_p, \mathcal{D}_p$. Since $T_p(\tau)$ in (242) can be multiplied by a τ-independent phase we may assume z to be real and positive. The solution of the Wronskian condition then gives

$$w = w_R - \frac{i}{2z}\,, \quad w_R,\, z > 0\,. \tag{246}$$

Inserting (246) into the above $\mathcal{E}$ one is led to minimize

$$\mathcal{E} = J\Big(w_R^2 + \frac{1}{4z^2}\Big) + Kz^2 - \dot{J}zw_R\,, \tag{247}$$

which gives

$$(z^{\min})^2 = \frac{J}{\sqrt{4KJ - \dot{J}^2}}\,, \quad w_R^{\min} = \frac{z^{\min}}{2}\frac{\dot{J}}{J}\,. \tag{248}$$

On general grounds the minimizer should be a zero of $\mathcal{D}$. Since

$$\frac{w^{\min}}{z^{\min}} = \frac{\dot{J}}{2J} - i\frac{\sqrt{4KJ - \dot{J}^2}}{2J}, \tag{249}$$

this is indeed the case. Reinserting (248) into $\mathcal{E}$ gives

$$\mathcal{E}^{\min} = \frac{1}{2}\sqrt{4KJ - \dot{J}^2}\,. \tag{250}$$

Since $\mathcal{E}$ in the original form (205) is manifestly non-negative this shows the selfconsistency of (245). The solution is unique up to a constant phase left undetermined by choosing $z > 0$. Upon insertion of (244) in (248), (249) the minimizing initial data become functionals of Δ, for which we write $z_p[\Delta](\tau_0) = z^{\min}$, $w_p[\Delta](\tau_0) = w^{\min}$. In summary

Theorem 5.2.2.

(a) A SLE can be characterized as a solution $|\psi;\tau\rangle_{\mathsf{s}}$ of the time dependent Schrödinger equation (210), (213) with initial data $|\psi;\tau_0\rangle_{\mathsf{s}}$ that minimize (for fixed window function f) the quantity $\int d\tau f(\tau)^2{}_{\mathsf{s}}\langle\psi;\tau|i\partial_\tau|\psi;\tau\rangle_{\mathsf{s}}$. The minimizing wave function is a Gaussian $\Omega_T[u]$ of the form (215) with $T = T^{\mathrm{SLE}}$, which is up to a time independent, potentially p dependent, phase uniquely determined by the commutator function.

(b) Specifically

$$\begin{aligned}
T_p^{\mathrm{SLE}}(\tau) &= \Delta_p(\tau,\tau_0)w_p[\Delta](\tau_0) - \partial_{\tau_0}\Delta_p(\tau,\tau_0)z_p[\Delta](\tau_0)\,,\\
z_p[\Delta](\tau_0) &= \sqrt{\frac{J_p(\tau_0)}{2\mathcal{E}_p^{\mathrm{SLE}}}} = T_p^{\mathrm{SLE}}(\tau_0)\,,\\
w_p[\Delta](\tau_0) &= \partial_{\tau_0}T_p^{\mathrm{SLE}}(\tau_0) - i\sqrt{\frac{\mathcal{E}_p^{\mathrm{SLE}}}{2J_p(\tau_0)}} = (\partial_\tau T_p^{\mathrm{SLE}})(\tau_0)\,,
\end{aligned} \tag{251}$$

where $J_p(\tau_0)$ is as in (244), and $\mathcal{E}_p^{\mathrm{SLE}}$ is the minimal energy given by

$$\begin{aligned}\big(\mathcal{E}_p^{\mathrm{SLE}}\big)^2 &= \frac{1}{8}\int d\tau d\tau' f(\tau)^2 f(\tau')^2 \Big\{ \big(\partial_\tau \partial_{\tau'} \Delta_p(\tau,\tau')\big)^2 + 2\omega_p(\tau')^2 (\partial_\tau \Delta_p(\tau',\tau))^2 \\ &+ \omega_p(\tau)^2 \omega_p(\tau')^2 \Delta_p(\tau,\tau')^2 \Big\}. \end{aligned} \tag{252}$$

For the modulus and the phase this gives

$$\big|T_p^{\mathrm{SLE}}(\tau)\big|^2 = \frac{J_p(\tau)}{2\mathcal{E}_p^{\mathrm{SLE}}}, \quad \tan\big(\arg T_p^{\mathrm{SLE}}(\tau)\big) = -\frac{\mathcal{E}_p^{\mathrm{SLE}} \Delta_p(\tau,\tau_0)}{J_p(\tau,\tau_0)}, \tag{253}$$

with

$$J_p(\tau,\tau_0) := \frac{1}{2}\int d\tau_1 \, f(\tau_1)^2 \big[\partial_{\tau_1}\Delta_p(\tau_1,\tau)\partial_{\tau_1}\Delta_p(\tau_1,\tau_0) + \omega_p(\tau_1)^2 \Delta_p(\tau_1,\tau)\Delta_p(\tau_1,\tau_0)\big]. \tag{254}$$

We note that $J_p(\tau_0)$ coincides with $J_p(\tau_0,\tau_0)$.

Proof.

(a) This follows from (214), (235), (237) and (222).

(b) Eq. (251) is the explicit form of (242) with minimizing parameters (248), (250). In the explicit expressions (253) with (252) and (254) a reduction of order occurs: where naively terms fourth or third order in Δ and its derivatives appear, repeated use of

$$\partial_{\tau_0}\Delta_p(\tau,\tau_0)\Delta_p(\tau',\tau_0) - \Delta_p(\tau,\tau_0)\partial_{\tau_0}\Delta_p(\tau',\tau_0) = \Delta_p(\tau,\tau'), \tag{255}$$

(as well as its ∂_τ, $\partial_{\tau'}$ and $\partial_\tau\partial_{\tau'}$ derivatives) leads to results merely quadratic in Δ and its derivatives. In detail, by inserting the definitions into $(\mathcal{E}_p^{\mathrm{SLE}})^2 = K_p(\tau_0)J_p(\tau_0) - (\partial_{\tau_0}J_p(\tau_0))^2/4$, one obtains an expression which is initially quartic in Δ. Repeated application of (255) then leads to (252). Since the right hand side of (252) is manifestly non-negative also the anticipated inequality (245) follows (without presupposing the minimization procedure). The result for the modulus-square follows from

$$K_p(\tau_0)\Delta(\tau,\tau_0)^2 + J_p(\tau_0)(\partial_{\tau_0}\Delta(\tau,\tau_0))^2 - \Delta(\tau,\tau_0)\partial_{\tau_0}\Delta(\tau,\tau_0)\partial_{\tau_0}J_p(\tau_0) = J_p(\tau) \tag{256}$$

and can be verified along similar lines. Finally, the ratio $\Im T_p^{\mathrm{SLE}}/\Re T_p^{\mathrm{SLE}}$ can be read off from (251) and gives the tan of the phase. Initially the ratio has as denominator the left hand

side of

$$2J_p(\tau_0)\partial_{\tau_0}\Delta_p(\tau_0,\tau)-\partial_{\tau_0}J_p(\tau_0)\Delta_p(\tau_0,\tau)=2J_p(\tau,\tau_0)\,. \tag{257}$$

The reduction of order occurs as before. □

Remarks:

(i) Modulo the dependence on the averaging function the expression (251) realizes the goal of constructing a Hadamard state solely from the state independent commutator function in a way different from [1, 17].

(ii) The parts (a) and (b) are logically independent and (b) can be obtained solely from minimizing $\mathcal{E}_p$ in (243). A minimization over initial data in the Heisenberg picture is however less compelling because for selfinteracting QFTs the fields (as operator valued distributions) do in general not admit a well-defined restriction to a sharp constant time hypersurface. On the other hand, the Schrödinger picture in QFT is frequently by default defined on a spatial lattice, see Proposition 5.2.1 here. The Gaussian (215) is then uniquely determined by the parameters $z_p = T_p(\tau_0)$, $w_p = (\partial_\tau T_p)(\tau_0)$ in its initial value $\Omega_T[u]|_{\tau=\tau_0}$. Conceptually, therefore (b) is naturally placed in the context of (a).

(iii) The relation $|T_p^{\mathrm{SLE}}(\tau)| \propto \sqrt{J_p(\tau)}$ also implies that $J(\tau)$ solves the Ermakov-Pinney equation with very specific f-dependent initial conditions implicitly set by those of Δ_p.

(iv) In terms of the data in (253) the SLE two-point function can be expressed as

$$\begin{aligned} &T_p^{\mathrm{SLE}}(\tau)T_p^{\mathrm{SLE}}(\tau')^* \\ &= \frac{\sqrt{J_p(\tau)J_p(\tau')}}{2\mathcal{E}_p^{\mathrm{SLE}}}\left(\frac{J_p(\tau,\tau_0)-i\mathcal{E}_p^{\mathrm{SLE}}\Delta_p(\tau,\tau_0)}{J_p(\tau,\tau_0)+i\mathcal{E}_p^{\mathrm{SLE}}\Delta_p(\tau,\tau_0)}\right)^{1/2}\left(\frac{J_p(\tau',\tau_0)+i\mathcal{E}_p^{\mathrm{SLE}}\Delta_p(\tau',\tau_0)}{J_p(\tau',\tau_0)-i\mathcal{E}_p^{\mathrm{SLE}}\Delta_p(\tau',\tau_0)}\right)^{1/2} \end{aligned} \tag{258}$$

(v) In principle, the equivalence of (251) to the original expression (227) is a consequence of the respective, independently established, uniqueness and the identity (222). It is nevertheless instructive to verify the equivalence of (251) and (227) directly. The main ingredient is the postponed proof of Proposition 5.2.2 to which we now turn.

We begin with a simple basic fact

Lemma 5.2.3. *Let $\Delta : C([\tau_i,\tau_f]) \to C([\tau_i,\tau_f]^2)$ be the following commutator functional*

$\Delta[S](\tau,\tau_0) = i(S(\tau)S(\tau_0)^* - S(\tau)^*S(\tau_0))$. *Then* $\Delta[S]$ *is real valued, antisymmetric in* τ,τ_0, *and obeys* $\Delta[aS+bS^*](\tau,\tau_0) = (|a|^2-|b|^2)\Delta[S](\tau,\tau_0)$, $a,b\in\mathbb{C}$. *On a solution* S *of the differential equation (193)* $\Delta[S]$ *becomes the commutator function, which is characterized by (201) and is independent of the choice of Wronskian normalized fiducial solution.*

Proof of Proposition 5.2.2.

We can regard $J_p(\tau_0), K_p(\tau_0)$ as functionals over the differentiable functions $C^1([\tau_i,\tau_f])$, by replacing the commutator function by the commutator functional $\Delta_p(\tau,\tau_0)\mapsto\Delta_p[S](\tau,\tau_0) = i(S(\tau)S(\tau_0)^*-S(\tau)^*S(\tau_0))$. Inserting this into (244) and comparing with the definitions (226) one finds

$$\begin{aligned} J_p(\tau_0) &= 2|S_p(\tau_0)|^2c_1 - [S_p(\tau_0)^*]^2c_2 - S_p(\tau_0)^2c_2^* = \mathcal{J}[S](\tau_0)\,,\\ K_p(\tau_0) &= 2|\partial_{\tau_0}S_p(\tau_0)|^2c_1 - [\partial_{\tau_0}S_p(\tau_0)^*]^2c_2 - [\partial_{\tau_0}S_p(\tau_0)]^2c_2^* = \mathcal{K}[S](\tau_0)\,. \end{aligned} \tag{259}$$

Using (259) one can compute the left hand side of (245) in terms of c_1,c_2. The result is

$$4K_p(\tau_0)J_p(\tau_0) - (\partial_{\tau_0}J_p(\tau_0))^2 = 4(c_1^2-|c_2|^2) = 4\mathcal{I}[S]\,. \tag{260}$$

Since $c_1\geq|c_2|$ this reconfirms (245). The invariance (229) of $\mathcal{I},\mathcal{J},\mathcal{K}$ follows from Lemma 5.2.3. □

Finally, we verify the equivalence of (251) and (227). For a general solution $T_p(\tau)$ one can match the parameterizations (223) and (242) by realizing the commutator function in terms of S. This gives

$$\begin{aligned} \lambda &= i\big(S_p(\tau_0)^*w - \partial_{\tau_0}S_p(\tau_0)^*z\big)\,,\\ \mu &= i\big(\partial_{\tau_0}S_p(\tau_0)z - S_p(\tau_0)w\big)\,. \end{aligned} \tag{261}$$

The same must hold for the minimizing parameters. A brute force verification of the latter is cumbersome. Instead we compare the modulus square computed from (224), i.e. $(|\mu|^2+|\lambda|^2)|S_p(\tau)|^2+\mu\lambda^*S(\tau)^2+\lambda\mu^*[S(\tau)^*]^2$ with $J_p(\tau)/(2\sqrt{c_1^2-|c_2|^2})$, taking advantage of the directly verified Eq. (256). Inserting (256) for $J_p(\tau)$ and comparing coefficients of $|S_p(\tau)|^2$,

$S_p(\tau)^2$, one finds

$$|\mu^{\min}|^2 + |\lambda^{\min}|^2 = \frac{c_1}{\sqrt{c_1^2 - |c_2|^2}}\,, \quad (\lambda^{\min})^* \mu^{\min} = -\frac{c_2^*}{2\sqrt{c_1^2 - |c_2|^2}}\,. \tag{262}$$

These can be solved for $\mu^{\min}, \lambda^{\min}$, and with the choice of phase $\arg \lambda^{\min} = \pi - \arg c_2$ one recovers (234). This provides a direct verification – modulo phase choices – of (261) for the minimizers (248) and (234). The phases are however not necessarily matched, in particular real μ does not automatically correspond to real z.

5.3 Convergent small momentum expansion for SLE

The SLE have been introduced on account of their Hadamard property, which relates to a Minkowski-like behavior at large spatial momentum. Here we show that SLE admit a convergent small momentum expansion, both for massive and for massless theories. Remarkably, the momentum dependence turns out to Minkowski-like also for small momentum. In the massless case this provides a cure for the infrared divergences plaguing the two-point functions on FL cosmologies with accelerated expansion. In fact, for any scale factor the leading terms are given by

$$T_p^{\mathrm{SLE}}(\tau)T_p^{\mathrm{SLE}}(\tau')^* = \frac{\bar{a}}{2p} - \frac{i}{2}(\tau-\tau') + O(p)\,, \quad \bar{a} := \left(\frac{\int d\tau f(\tau)^2}{\int d\tau f(\tau)^2 a(\tau)^{2d-2}}\right)^{\frac{1}{2}}. \tag{263}$$

5.3.1 Fiducial solutions and their Cauchy product

A SLE can be defined either in terms of a fiducial solution S_p or in terms of the Commutator function Δ_p. Here we prepare results establishing uniformly convergent series for these solutions as well as their Cauchy products. Throughout we consider the differential equation

$$[\partial_\tau^2 + \omega_p(\tau)^2]S_p(\tau) = 0\,, \quad \omega_p(\tau)^2 = \omega_0(\tau)^2 + p^2\omega_2(\tau)^2\,, \tag{264}$$

where ω_0, ω_2 are continuous real-valued functions on $[\tau_i, \tau_f]$ and ω_2 is not identically zero. The case $\omega_0(\tau)^2 = m(\tau)^2 a(\tau)^{2d}$, $\omega_2(\tau)^2 = a(\tau)^{2d-2}$ corresponds to the dispersion relation arising from the Klein Gordon equation; the function $m(\tau)$ may have zeros or vanish identically (massless case). Throughout we write p for the modulus of the spatial momentum.

Proposition 5.3.1. The differential equation (264) admits convergent series solutions with a radius of convergence $p_* > 0$ on $[\tau_i, \tau_f]$, such that for any $p < p_*$

$$S_p(\tau) \;=\; \sum_{n=0}^{\infty} S_n(\tau)p^{2n}\,, \quad \text{and} \quad \partial_\tau S_p(\tau) = \sum_{n=0}^{\infty} \partial_\tau S_n(\tau)p^{2n}\,, \tag{265}$$

and the sums converge *uniformly* on $[\tau_i, \tau_f]$.

These solutions in particular have IR finite initial data

$$\lim_{p\to 0} S_p(\tau_0) =: z_0 < \infty\,, \quad \lim_{p\to 0} \partial_{\tau_0} S_p(\tau_0) =: w_0 < \infty\,. \tag{266}$$

The proof below entails that the subspace of solutions described by the proposition can be characterized by (266). In order to prove the proposition, we shall need the following standard existence and uniqueness result for the solutions of a second order linear ODE (which we state without proof):

Lemma 5.3.1. *Consider the initial value problem*

$$y''(\tau) + \alpha(\tau)y'(\tau) + \beta(\tau)y(\tau) = g(\tau)\,, \quad y(\tau_0) = u\,,\ y'(\tau_0) = v\,. \tag{267}$$

If α, β, g are continuous functions on an open interval $I \ni \tau_0$, then there exists a unique solution of this initial value problem, and this solution exists throughout the interval I.

Proof of Proposition 5.3.1.

First consider the "$p = 0$" equation, *i.e.* $[\partial_\tau^2 + \omega_0(\tau)^2]S_0(\tau) = 0$. Lemma 5.3.1 implies that there exists a complex solution $S_0(\tau)$, which may be Wronskian normalized to satisfy $\partial_\tau S_0\, S_0^* - S_0 \partial_\tau S_0^* = -i$. In the case $\omega_0(\tau) = 0$ on $[\tau_i,\, \tau_f]$, the solution with initial data w_0, z_0 is $S_0(\tau) = w_0(\tau - \tau_0) + z_0$, $w_0 z_0^* - z_0 w_0^* = -i$. Remaining with general $\omega_0(\tau)$ we reformulate (264) as an integral equation. Defining the kernel[1]

$$K(\tau,\, \tau') := i\theta(\tau - \tau')S_0(\tau)S_0(\tau')^* + i\theta(\tau' - \tau)S_0(\tau)^* S_0(\tau')\,, \tag{268}$$

a function $S(\tau)$ satisfying

$$S(\tau) \;=\; S_0(\tau) - p^2 \int_{\tau_i}^{\tau_f} K(\tau,\, \tau')\omega_2(\tau')^2 S(\tau') d\tau' \tag{269}$$

solves (264). Further, $\partial_\tau S(\tau)$ satisfies

$$\partial_\tau S(\tau) = \partial_\tau S_0(\tau) - p^2 \int_{\tau_i}^{\tau_f} \partial_\tau K(\tau, \tau')\omega_2(\tau')^2 S(\tau') d\tau'\,. \tag{270}$$

[1]This is the (generalized) Feynman Greens function. Any other choice of Greens function also renders L in (273) a contraction, merely the value of p_* may change.

In terms of

$$\mathcal{S}(\tau) := \begin{pmatrix} S(\tau) \\ \tilde{S}(\tau) \end{pmatrix}, \quad \mathcal{S}_0(\tau) := \begin{pmatrix} S_0(\tau) \\ \partial_\tau S_0(\tau) \end{pmatrix}, \quad \mathcal{K}(\tau,\tau') := \begin{pmatrix} K(\tau,\,\tau')\omega_2(\tau')^2 & 0 \\ \partial_\tau K(\tau,\tau')\omega_2(\tau')^2 & 0 \end{pmatrix}, \tag{271}$$

we search for a solution of the integral equation

$$\mathcal{S}(\tau) = \mathcal{S}_0(\tau) - p^2 \int_{\tau_i}^{\tau_f} \mathcal{K}(\tau,\tau')\mathcal{S}(\tau')d\tau' \,. \tag{272}$$

As the underlying Banach space we take $(X, \|\cdot\|) := \big(C([\tau_i,\tau_f],\mathbb{C}^2), \|\cdot\|_{\sup}\big)$, where $\mathbb{C}^2$ is being equipped with the sup-norm. Next, we define the linear operator $L : X \to X$

$$\forall\, u \in X :\ \big(Lu\big)(\tau) := \mathcal{S}_0(\tau) - p^2 \int_{\tau_i}^{\tau_f} \mathcal{K}(\tau,\,\tau')u(\tau')d\tau' \,, \tag{273}$$

and show that for sufficiently small p, this map is actually a contraction.

Since S_0 is a C^1 function, it is clear that both $K(\tau,\tau')$ and $\partial_\tau K(\tau,\tau')$ are bounded functions on $[\tau_i,\tau_f]^2$. As ω_2 is also continuous, there is $R > 0$ such that $|\mathcal{K}(\tau,\tau')_{ij}| < R$ on $[\tau_i,\tau_f]^2$. Then for any $u,\, v \in X$

$$\begin{aligned} |Lu(\tau) - Lv(\tau)|_{\max} &= p^2 \Big| \int_{\tau_i}^{\tau_f} \mathcal{K}(\tau,\tau')\big(u(\tau') - v(\tau')\big)d\tau' \Big|_{\max} \\ &\le p^2 \int_{\tau_i}^{\tau_f} \Big| \mathcal{K}(\tau,\tau')\big(u(\tau') - v(\tau')\big) \Big|_{\max} d\tau' \\ \implies \|Lu - Lv\|_{\sup} &\le p^2(\tau_f - \tau_i)R\, \|u - v\|_{\sup} \,, \end{aligned} \tag{274}$$

and so there is $p_* > 0$ such that for all $p < p_*$, L is a contraction.

Assuming that $p < p_*$, the Banach Fixed Point theorem implies that there exists a *unique* $\mathcal{S}_p = (S_p,\, \tilde{S}_p)^T \in X$ such that $L\mathcal{S}_p = \mathcal{S}_p$, *i.e.*

$$\begin{aligned} S_p(\tau) &= S_0(\tau) - p^2 \int_{\tau_i}^{\tau_f} K(\tau,\,\tau')\omega_2(\tau')^2 S_p(\tau')d\tau' \,, \\ \tilde{S}_p(\tau) &= \partial_\tau S_0(\tau) - p^2 \int_{\tau_i}^{\tau_f} \partial_\tau K(\tau,\,\tau')\omega_2(\tau')^2 S_p(\tau')d\tau' \,. \end{aligned} \tag{275}$$

Comparing (275) and (270), it is clear that $\partial_\tau S_p(\tau)$ satisfies the second equation above. The uniqueness of the fixed point $\mathcal{S}_p$ then implies that $\tilde{S}_p = \partial_\tau S_p$.

Further, the iterated sequence $L^m\mathcal{S}_0$, $m \in \mathbb{N}$, converges to $\mathcal{S}_p$ in the sup-norm. It is then

easily verified that there is a sequence of C^1 functions $S_n(\tau)$ such that we have the *uniformly convergent* power series representations of the form asserted in (265). □

Next we consider the product of two series solutions and state, without proof, the following slight generalization of Merten's theorem.

Lemma 5.3.2. *Let*

$$A(\tau) = \sum_{n=0}^{\infty} a_n(\tau) p^{2n}\,, \quad B(\tau) = \sum_{n=0}^{\infty} b_n(\tau) p^{2n}\,, \tag{276}$$

be power series in the Banach space $C([\tau_i, \tau_f], \mathbb{C})$ with (uniform) radius of convergence $p_* > 0$. Consider the map $C : [\tau_i, \tau_f] \times [\tau_i, \tau_f] \to \mathbb{C}$ defined by $C(\tau_1, \tau_2) := A(\tau_1)B(\tau_2)$, and the coefficients of the unequal time Cauchy product of A and B,

$$c_n(\tau_1, \tau_2) \;\; := \;\; \sum_{i=0}^{n} a_i(\tau_1) b_{n-i}(\tau_2)\,. \tag{277}$$

Then for any $p < p_*$

$$\sum_{n=0}^{\infty} c_n(\tau_1, \tau_2) p^{2n} \;\; = \;\; C(\tau_1, \tau_2)\,, \tag{278}$$

with uniform convergence in $[\tau_i, \tau_f] \times [\tau_i, \tau_f]$. The same holds for the equal time Cauchy product ($\tau_1 = \tau_2$ in (277), (278)) with uniform convergence in $[\tau_i, \tau_f]$.

An immediate corollary of Proposition 5.3.1 and Lemma 5.3.2 is:

Corollary 5.3.3. *The Commutator function $\Delta_p(\tau, \tau')$ and the Greens functions defined in terms of it have uniformly convergent series expansions in $p < p_*$ for distinct $(\tau, \tau') \in [\tau_i, \tau_f] \times [\tau_i, \tau_f]$.*

So far these are mostly existence results. For the actual construction of these series solutions one will solve the implied recursion relations. For a solution $S_p(\tau)$ of the form (265) one has

$$\begin{aligned} [\partial_\tau^2 + \omega_0(\tau)^2] S_0(\tau) \;\; &= \;\; 0\,, \\ [\partial_\tau^2 + \omega_0(\tau)^2] S_n(\tau) \;\; &= \;\; -\omega_2(\tau)^2 S_{n-1}(\tau)\,, \quad n \geq 1\,. \end{aligned} \tag{279}$$

Each S_n is only unique up to addition of a solution of the homogeneous equation, characterized by two complex parameters. These ambiguities account for the initial data of the series solution

$$S_p(\tau_0) = \sum_{n\geq 0} z_n p^{2n} =: z_p\,, \quad \partial_{\tau_0} S_p(\tau_0) = \sum_{n\geq 0} w_n p^{2n} =: w_p\,,$$
$$\text{with} \quad \sum_{j=0}^{n} (w_j z^*_{n-j} - w^*_j z_{n-j}) = 0\,, \quad n \geq 1\,, \tag{280}$$

where the constraint stems from the Wronskian normalization. One can use the same Greens function $G_0(\tau', \tau)$ at each order and adjust the initial data of the additive modification such that $S_n(\tau_0) = z_n$, $(\partial_\tau S_n)(\tau_0) = w_n$ holds, for given $z_n, w_n \in \mathbb{C}$, mildly constrained by (280).

Later on a series solution of this form will play the role of the fiducial solution in the construction of the SLE. Theorem 5.2.1 ensures that *any* such solution will produce the *same* SLE solution (within the implied radius of convergence) up to a phase. We are therefore free to choose one with especially simple, namely p-independent, initial data for $\tau_0 = \tau_i$: $z_n = 0 = w_n$, $n \geq 1$. In this case the relevant Greens function is the retarded Greens function $G_0^\wedge(\tau, \tau') := \theta(\tau - \tau')\Delta_0(\tau, \tau')$, with Δ_0 the commutator function for $\partial_\tau^2 + \omega_0(\tau)^2$. Further, no additive, order dependent, modification is needed and the solution of the iteration is simply

$$\begin{aligned} S_n(\tau) \;&=\; \int_{\tau_i}^{\tau_f} d\tau'\, K_n(\tau, \tau')\, S_0(\tau')\,, \quad n \geq 1\,, \\ K_1(\tau, \tau') \;&:=\; -G_0^\wedge(\tau, \tau')\omega_2(\tau')^2\,, \\ K_{n+1}(\tau, \tau') \;&:=\; (-)^{n+1} \int_{\tau_i}^{\tau_f} d\tau_1 ... d\tau_n\, G_0^\wedge(\tau, \tau_1)\omega_2(\tau_1)^2\, G_0^\wedge(\tau_1, \tau_2)\omega_2(\tau_2)^2 \dots\, G_0^\wedge(\tau_n, \tau')\omega_2(\tau')^2\,. \end{aligned} \tag{281}$$

The kernel K_n is manifestly real and satisfies $K_n(\tau_i, \tau') = 0 = \partial_\tau K_n(\tau, \tau')|_{\tau=\tau_i}$, for $\tau' \in (\tau_i, \tau_f]$. The associated series solution $S_p(\tau)$ therefore satisfies $S_p(\tau_i) = z_0$, $(\partial_\tau S_p)(\tau_i) = w_0$, for p-independent constants with $w_0 z_0^* - w_0^* z_0 = -i$.

The commutator function $\Delta_p(\tau, \tau')$ is likewise independent of the choice of the Wronskian normalized solution used to realize it, see Lemma 5.2.3. We are thus free to use the solution

(281) for this purpose. Writing $\Delta_p(\tau,\tau') = \sum_{n\geq 0} \Delta_n(\tau,\tau')p^{2n}$, one finds

$$\begin{aligned}
\Delta_n(\tau,\tau') &= i\sum_{j=0}^{n} \big(S_j(\tau)S^*_{n-j}(\tau') - S^*_j(\tau)S_{n-j}(\tau')\big) \\
&= \int_{\tau_i}^{\tau_f} ds[K_n(\tau,s)\Delta_0(s,\tau') - K_n(\tau',s)\Delta_0(s,\tau)] \\
&+ \int_{\tau_i}^{\tau_f} ds_1 ds_2 \sum_{j=1}^{n-1} K_j(\tau,s_1)K_{n-j}(\tau',s_2)\Delta_0(s_1,s_2)\,. \qquad (282)
\end{aligned}$$

One can check that the coefficients satisfy all the relations implied by the expansion of the defining conditions (201)

$$\begin{aligned}
[\partial_\tau^2 + \omega_0(\tau)^2]\Delta_n(\tau,\tau') &= -\omega_2(\tau)^2\Delta_{n-1}(\tau,\tau')\,, \quad \partial_\tau\Delta_n(\tau,\tau')\big|_{\tau=\tau'} = 0\,, \\
[\partial_{\tau'}^2 + \omega_0(\tau')^2]\Delta_n(\tau,\tau') &= -\omega_2(\tau')^2\Delta_{n-1}(\tau,\tau')\,, \quad n\geq 1\,. \qquad (283)
\end{aligned}$$

The two recursion relations follow from $[\partial_\tau^2 + \omega_0(\tau)^2]K_n(\tau,\tau') = -\omega_2(\tau)^2 K_{n-1}(\tau,\tau')$, $n\geq 2$. For the third relation it is convenient to first verify $\partial_\tau[\partial_\tau\Delta_n(\tau,\tau')|_{\tau=\tau'}] = 0$. Then, it suffices to show $\partial_\tau\Delta_n(\tau,\tau_i)|_{\tau=\tau_i} = 0$, which follows from $K_n(\tau_i,\tau') = 0 = \partial_\tau K_n(\tau,\tau')|_{\tau=\tau_i}$, for $\tau'\in(\tau_i,\tau_f]$.

5.3.2 IR behavior of States of Low Energy

We use the formulas from Theorem 5.2.2 to derive convergent series expansions for the SLE. The basic expansion is $\Delta_p(\tau',\tau) = \sum_{n\geq 0}\Delta_n(\tau',\tau)p^{2n}$, with coefficients from (282). In terms of it convergent expansions for the $J_p(\tau_0), \partial_{\tau_0}J_p(\tau_0), K_p(\tau_0)$ in (244) can be derived. The uniform convergence of the various pointwise products is ensured by the results of Section 5.3.1 and allows one to exchange the order of summation and integration. The following notation is convenient

$$\begin{aligned}
&C(\tau,\tau_0) = \sum_{n\geq 0} C_n(\tau,\tau_0)\,p^{2n} \quad \Longrightarrow \quad C(\tau,\tau_0)^2 = \sum_{n\geq 0} C(\tau,\tau_0)^2_n\,p^{2n} \\
&\text{with} \quad C(\tau,\tau_0)^2_n := \sum_{j=0}^{n} C_j(\tau,\tau_0)C_{n-j}(\tau,\tau_0)\,. \qquad (284)
\end{aligned}$$

In this notation one has

$$
\begin{aligned}
J_p(\tau_0) &= \sum_{n\geq 0} J_n(\tau_0)\, p^{2n}\,, \qquad K_p(\tau_0) = \sum_{n\geq 0} K_n(\tau_0)\, p^{2n}\,, \\
J_0(\tau_0) &= \frac{1}{2}\int d\tau\, f(\tau)^2 \Big[\big(\partial_\tau \Delta_0(\tau,\tau_0)\big)^2 + \omega_0(\tau)^2 \Delta_0(\tau,\tau_0)^2 \Big]\,, \\
J_n(\tau_0) &= \frac{1}{2}\int d\tau\, f(\tau)^2 \Big[\big(\partial_\tau \Delta(\tau,\tau_0)\big)_n^2 + \omega_0(\tau)^2 \Delta(\tau,\tau_0)_n^2 + \omega_2(\tau)^2 \Delta(\tau,\tau_0)_{n-1}^2 \Big]\,, \\
K_0(\tau_0) &= \frac{1}{2}\int d\tau\, f(\tau)^2 \Big[\big(\partial_\tau \partial_{\tau_0} \Delta_0(\tau,\tau_0)\big)^2 + \omega_0(\tau)^2 \big(\partial_{\tau_0} \Delta_0(\tau,\tau_0)\big)^2 \Big]\,, \\
K_n(\tau_0) &= \frac{1}{2}\int d\tau\, f(\tau)^2 \Big[\big(\partial_\tau \partial_{\tau_0} \Delta(\tau,\tau_0)\big)_n^2 + \omega_0(\tau)^2 \big(\partial_{\tau_0} \Delta(\tau,\tau_0)\big)_n^2 + \omega_0(\tau)^2 \big(\partial_{\tau_0} \Delta(\tau,\tau_0)\big)_{n-1}^2 \Big]\,,
\end{aligned}
\tag{285}
$$

and $\partial_{\tau_0} J_p(\tau_0) = \sum_{n\geq 0} \partial_{\tau_0} J_n(\tau,\tau_0)\, p^{2n}$ with the implied coefficients. Interpreting (252) as

$$
\begin{aligned}
(\mathcal{E}_p^{\mathrm{SLE}})^2 &= \frac{1}{4}\int d\tau_0 f(\tau_0)^2 \big[K_p(\tau_0) + \omega_p(\tau_0)^2 J_p(\tau_0) \big] =: \sum_{n\geq 0} \varepsilon_n^2\, p^{2n}\,, \\
\varepsilon_0^2 &= \frac{1}{4}\int d\tau_0 f(\tau_0)^2 \big[K_0(\tau_0) + \omega_0(\tau_0)^2 J_0(\tau_0) \big]\,, \\
\varepsilon_n^2 &= \frac{1}{4}\int d\tau_0 f(\tau_0)^2 \big[K_n(\tau_0) + \omega_0(\tau_0)^2 J_n(\tau_0) + \omega_2(\tau_0)^2 J_{n-1}(\tau_0) \big]\,, \quad n \geq 1\,,
\end{aligned}
\tag{286}
$$

one sees that the energy's expansion is determined by the same coefficients. As a consequence all quantities in Theorem 5.2.2(b) admit convergent series expansions in powers of p whose coefficients can be expressed in terms of those in (285) only.

In the following we focus on the expansion of the energy $\mathcal{E}_p^{\mathrm{SLE}}$ and the modulus squared $|T_p^{\mathrm{SLE}}(\tau)|^2$. It is useful to distinguish two cases (where the terminology will become clear momentarily).

Massive: $\varepsilon_0 > 0$ and $K_0(\tau_0) > 0$.

$$
\begin{aligned}
\mathcal{E}_p^{\mathrm{SLE}} &= \varepsilon_0 + \frac{\varepsilon_1^2}{2\varepsilon_0} p^2 - \frac{\varepsilon_1^4 - 4\varepsilon_0^2\varepsilon_2^2}{8\varepsilon_0^3} p^4 + O(p^6)\,, \\
|T_p^{\mathrm{SLE}}(\tau)|^2 &= \frac{J_0(\tau)}{2\varepsilon_0} + \frac{2J_1(\tau)\varepsilon_0^2 - J_0(\tau)\varepsilon_1^2}{4\varepsilon_0^3} p^2 \\
&\quad + \frac{1}{16\varepsilon_0^5}\big(8J_2(\tau)\varepsilon_0^4 - 4J_1(\tau)\varepsilon_0^2\varepsilon_1^2 + 3J_0(\tau)\varepsilon_1^4 - 4J_0(\tau)\epsilon_0^2\varepsilon_2^2\big) p^4 + O(p^6)\,.
\end{aligned}
\tag{287}
$$

Massless: $\varepsilon_0 = 0$ and $K_0(\tau_0) = 0$ and $\varepsilon_1 > 0$.

$$\begin{aligned}
\mathcal{E}_p^{\rm SLE} &= \varepsilon_1 p + \frac{\varepsilon_2^2}{2\varepsilon_1} p^3 - \frac{\varepsilon_2^4 - 4\varepsilon_1^2\varepsilon_3^2}{8\varepsilon_1^3} p^5 + O(p^7)\,, \\
|T_p^{\rm SLE}(\tau)|^2 &= \frac{J_0(\tau)}{2\varepsilon_1}\frac{1}{p} + \frac{2J_1(\tau)\varepsilon_1^2 - J_0(\tau)\varepsilon_2^2}{4\varepsilon_1^3} p \\
&+ \frac{1}{16\varepsilon_1^5}\big(8J_2(\tau)\varepsilon_1^4 - 4J_1(\tau)\varepsilon_1^2\varepsilon_2^2 + 3J_0(\tau)\varepsilon_2^4 - 4J_0(\tau)\epsilon_1^2\varepsilon_3^2\big)p^3 + O(p^5)\,.
\end{aligned} \tag{288}$$

The massive case corresponds to $\omega_0(\tau) = m(\tau)^2 a(\tau)^{2d}$, $\omega_2(\tau)^2 = a(\tau)^{2d-2}$. Even the lowest order commutator function $\Delta_0(\tau,\tau')$ can then in general no longer be found in closed form. All other aspects of the expansions are however explicitly computable in terms of Δ_0: the Δ_n's via (282), the J_n, K_n's via (285), the ε_n's from (286), and hence everything else.

Two-point function of massless SLE:

The massless case corresponds to $\omega_0(\tau) = 0$, $\omega_2(\tau)^2 = a(\tau)^{2d-2}$. The lowest order wave equation in (279) is then trivially soluble: $S_0(\tau) = w_0(\tau - \tau_0) + z_0$, with $w_0 z_0^* - w_0^* z_0 = -i$. The coefficients of the commutator function are explicitly known

$$\begin{aligned}
\Delta_0(\tau',\tau) &= \tau' - \tau\,, \\
\Delta_1(\tau',\tau) &= \int_{\tau_i}^{\tau_f} ds[\theta(\tau - s) - \theta(\tau' - s)](\tau - s)(\tau' - s)a(s)^{2d-2}\,,
\end{aligned} \tag{289}$$

etc. This entails $K_0(\tau_0) = 0$, $\varepsilon_0 = 0$, and

$$\begin{aligned}
\varepsilon_1^2 &= \frac{1}{4}\int d\tau f(\tau)^2 \int d\tau' f(\tau')^2 a(\tau')^{2d-2}\,, \\
J_0(\tau_0) &= \frac{1}{2}\int d\tau f(\tau)^2\,, \quad J_1(\tau_0) = \int d\tau f(\tau)^2\big[\partial_\tau \Delta_1(\tau,\tau_0) + (\tau - \tau_0)^2 a(\tau)^{2d-2}\big]\,, \\
K_1(\tau_0) &= \frac{1}{2}\int d\tau f(\tau)^2 a(\tau)^{2d-2}\,.
\end{aligned} \tag{290}$$

This gives

$$|T_p^{\rm SLE}(\tau)|^2 = \frac{\bar{a}}{2p} + O(p)\,, \quad \mathcal{E}_p^{\rm SLE} = \frac{p}{2\bar{a}}\int d\tau f(\tau)^2\,, \quad \bar{a} := \left(\frac{\int d\tau f(\tau)^2}{\int d\tau f(\tau)^2 a(\tau)^{2d-2}}\right)^{\frac{1}{2}}, \tag{291}$$

as claimed in (263). Since the leading term is τ independent one obtains from (251)

$$T_p^{\rm SLE}(\tau) = \Delta_p(\tau,\tau_0) w_p^{\min} - \partial_{\tau_0}\Delta_p(\tau,\tau_0) z_p^{\min} = \sqrt{\frac{\bar{a}}{2p}} - i(\tau - \tau_0)\sqrt{\frac{p}{2\bar{a}}} + O(p^{3/2})\,.$$

$$z_p^{\min} \;=\; \sqrt{\frac{\bar{a}}{2p}}\Big(1+O(p^2)\Big)\,, \quad w_p^{\min} = -i\sqrt{\frac{p}{2\bar{a}}}\Big(1+O(p^2)\Big)\,. \tag{292}$$

This holds up an undetermined p-dependent phase which is fixed in the initial value formulation of the minimization procedure by taking z real. This phase ambiguity disappears in the two-point function, for which one obtains

$$T_p^{\rm SLE}(\tau)T_p^{\rm SLE}(\tau')^* = \frac{\bar{a}}{2p} - \frac{i}{2}(\tau-\tau') + O(p)\,. \tag{293}$$

The same result can alternatively be obtained from (258).

Remarks:

(i) Based on (perhaps misled by) the exactly soluble case of power-like scale factors one normally regards the IR behavior of the solutions as directly determined by the cosmological scale factor. From the small argument expansion of the Bessel functions one has

$$|S_p(\tau)|^2 \propto p^{-2|\nu|} \quad \text{for} \quad a(\tau) \propto \tau^{\frac{1-2\nu}{2(d-1)\nu}}\,. \tag{294}$$

Here $d/2 < \nu < \infty$ corresponds to acceleration while $-\infty < \nu < 1/2$ corresponds to deceleration. The interval $1/2 \leq \nu \leq d/2$ does not give rise to a curvature singularity; the boundary values $\nu = 1/2$ and $\nu = d/2$ model Minkowski space and deSitter space, respectively. The inverse Fourier transform is infrared finite whenever $\int_0^1 dp\, p^{d-1}|S_p(\tau)|^2$ is finite. For the solutions (294) this is the case only in part of the decelerating window, $0 < \nu < 1/2$, see [37] for the original discussion.

(ii) The leading IR behavior of the massless SLE solution (292) is constant, pointwise in τ. This corresponds to the expected freeze-out of the oscillatory behavior on scales much larger than the Hubble radius. The universality of the $1/\sqrt{p}$ behavior is however surprising, as is the simple coefficient $\sqrt{\bar{a}/2}$, valid for *any* scale factor. The result (292) could not have been obtained based on the traditional adiabatic iteration, which is incurably singular at small momentum.

(iii) In arriving at (292) we took the expressions from Theorem 5.2.2 as the starting point. It is instructive to go through the derivation based on the original parameterization (223), (225). The fiducial solution is constructed via (281) from its leading order, S_0. In the massless case the general (Wronskian normalized) solution to the leading order equation is

$S_0(\tau) = w_0(\tau-\tau_0) + z_0$, $w_0 z_0^* - w_0^* z_0 = -i$. A somewhat longer computation then gives

$$\begin{aligned}
\mu_p &= |w_0|\sqrt{\frac{\bar{a}}{2p}} - \frac{1}{|w_0|}\sqrt{\frac{p}{8\bar{a}}} + O(p^{\frac{3}{2}})\,, \\
\lambda_p &= -\frac{w_0^*}{w_0}|w_0|\sqrt{\frac{\bar{a}}{2p}} - \frac{w_0^*}{w_0}\frac{1}{|w_0|}\sqrt{\frac{p}{8\bar{a}}} + O(p^{\frac{3}{2}})\,. \qquad (295) \\
T_p^{\mathrm{SLE}}(\tau) &= -i\frac{w_0^*}{|w_0|}\sqrt{\frac{\bar{a}}{2p}} - \frac{1}{|w_0|w_0}\sqrt{\frac{p}{8\bar{a}}}\Big[2|w_0|^2(\tau-\tau_0) + 2\Re(z_0 w_0^*)\Big] + O(p^{\frac{3}{2}})\,.
\end{aligned}$$

One sees that all intermediate results depend on the parameters w_0, z_0 of the fiducial solution. In the two-point function, however, these drop out and one recovers (293).

(iv) While in the massive case minimization of $\mathcal{E}_p$ and expansion in p^2 are commuting operations, this is not true in the massless case. In the SLE construction via a fiducial solution we chose one with a regular $p \to 0$ limit, which is evidently not the case for (292). The independence of the SLE solution from the choice of fiducial solution is crucial for the result.

(v) The IR behavior of (293) is Minkowski-like for *all* scale factors a. This means that massless SLE are automatically IR finite and provide an elegant solution to the long standing IR divergences in Friedmann-Lemaître backgrounds with accelerated expansion [37].

(vi) The existence of a pre-inflationary epoch with non-accelerated expansion typically removes the IR singularity. For generic powerlike scale factors the mode matching can (with some effort) be controlled analytically [55]; typically one focuses on a radiation dominated ($\nu = -1/2$ in (294)) [25, 71] or kinetic energy dominated ($\nu = 0$ in (294)) [23, 86] pre-inflationary period. Another take on the IR issue is to regard it as an artifact of using non-gauge invariant observables [51, 39].

(vii) The mathematical principle underlying (293) is very different from the ones in (vi). As detailed in Section 5.5, there are independent reasons to regard the existence of a pre-inflationary period as part of the standard paradigm. Positing a massless SLE as primordial vacuum in this period then ought to be consistent with the qualitative properties of the power spectrum at seed formation. This physics requirement will be taken up in Section 5.5.2.

(viii) As a consequence of (293) the long range properties of the SLE position space

two-point function will be similar to that of its Minkowski space counterpart. Further, the shift symmetry, $\phi(\tau, x) \mapsto \phi(\tau, x) + \text{const}$, turns out to be spontaneously broken for $d \geq 2$, as it is for the massless free field in Minkowski space. A proper proof can be based on Swieca's Noether charge criterion [57, 67] and is omitted here.

5.4 WKB type large momentum asymptotics

Any Wronskian normalized solution of the basic wave equation is uniquely determined by its modulus

$$S_p(\tau) = |S_p(\tau)| \exp\Big\{ -\frac{i}{2} \int_{\tau_0}^{\tau} ds \frac{1}{|S_p(s)|^2} \Big\}, \tag{296}$$

up to a choice of τ_0 where $S_p(\tau_0)$ is real. In this section we show that for each $N > 1$ there exists an exact 'order N' solution with a certain N-term positive frequency asymptotics. These solutions are such that $|S_p(\tau)|^2$ is asymptotic up to $O(p^{-2N-1})$ to a polynomial in odd inverse powers of p, whose coefficients are *local* differential polynomials in ω_0, ω_2 generalizing the heat kernel coefficients. The resulting order N solutions will be referred to as WKB type solutions.[2] An SLE solution will then be shown to be a WKB type solution of *infinite* order. Throughout this section we assume ω_0, ω_2 to be smooth.

5.4.1 Existence of solutions with WKB type asymptotics

As a starting point the relation (296) is cumbersome because the exponential needs to be re-expanded. In the following we establish the existence of asymptotic expansions of all quantities needed by starting from a simplified formal series ansatz for S_p's large momentum asymptotics

$$S_p(\tau) = \frac{\exp\big\{ -ip \int_{\tau_i}^{\tau} ds\, \omega_2(s) \big\}}{\sqrt{2p\omega_2(\tau)}} \Big\{ 1 + \sum_{n \geq 1} (ip)^{-n} s_n(\tau) \Big\}, \tag{297}$$

[2] A WKB ansatz proper is one where only the integrand of the exponent is formally expanded in terms of local coefficients.

with real-valued s_n. As in Section 5.3 we consider the basic differential equation $[\partial_\tau^2 + \omega_p(\tau)^2]S_p(\tau) = 0$ with generic time dependent frequency $\omega_p(\tau) = \omega_0(\tau)^2 + p^2\omega_2(\tau)^2$. The leading term in (297) is a positive frequency wave. The latter is known to be a necessary (but by no means sufficient property) for a solution to comply with the Hadamard condition.

Upon insertion of (297) into the basic wave equation one finds the following recursion relations

$$\begin{aligned} \partial_\tau s_n &= \partial_\tau s_1 s_{n-1} + \partial_\tau\Big(\frac{\partial_\tau s_{n-1}}{2\omega_2}\Big)\,, \quad n \geq 2\,, \\ \partial_\tau s_1 &= \frac{\omega_0^2}{2\omega_2} - \frac{1}{4\omega_2}\bigg(\frac{\partial_\tau^2\omega_2}{\omega_2} - \frac{3}{2}\Big(\frac{\partial_\tau\omega_2}{\omega_2}\Big)^2\bigg)\,. \end{aligned} \tag{298}$$

Clearly, each s_n can be obtained simply by integration and the only ambiguity arises from the choice of integration constants $s_n(\tau_i)$. We claim that

$$s_n(\tau_i) = 0\,, \quad n \text{ odd}\,, \tag{299}$$

uniquely determines all $s_n(\tau_i)$, n even, such that the Wronskian normalization condition holds. The stipulation $s_n(\tau_i) = 0$, n odd, goes hand in hand with the fact (seen later on) that $|S_p(\tau)|^2$ admits an asymptotic expansion in odd inverse powers of p. Comparing with the $|S_p(\tau_i)|^2$ series arising from (297) one sees that the odd s_n must vanish at $\tau = \tau_i$. The stipulation is also consistent with the flat space limit $a(\tau) \equiv 1$.

The second part of the claim is that the $s_n(\tau_i)$ for n even are determined by imposing the Wronskian normalization condition

$$\partial_\tau S_p(\tau) S_p(\tau)^* - S_p(\tau)\partial_\tau S_p(\tau)^* \stackrel{!}{=} -i\,. \tag{300}$$

Using momentarily a '$\prime$' to denote a ∂_τ derivative and setting $s_0 := 1$, a formal computation shows (300) to hold subject to (299) iff

$$\sum_{m,\,n\geq 0\,,m+n=N} (s_{2n}s_{2m})(\tau_i) - \sum_{m\geq 0,\,n\geq 1,\,2m+n=2N-1} (\omega_2^{-1}s_n'\,s_{2m})(\tau_i) \stackrel{!}{=} 0\,, \quad N \geq 1\,. \tag{301}$$

To low orders,

$$N = 1: \quad 2s_2(\tau_i) - \omega_2(\tau_i)^{-1}s_1'(\tau_i) \stackrel{!}{=} 0$$

$$N=2: \quad 2s_4(\tau_i)+s_2(\tau_i)^2-\omega_2(\tau_i)^{-1}s_3'(\tau_i)-\omega_2^{-1}s_1'(\tau_i)s_2(\tau_i)\stackrel{!}{=}0\,. \tag{302}$$

Clearly, $s_2(\tau_i)$ is determined by the unambiguous $s_1'(\tau_i)$ from (298). In terms of it $s_4(\tau_i)$ is determined by the unambiguous $s_3'(\tau_i)$, and so forth. Hence (301) iteratively fixes the integration constants $s_n(\tau_i)$ for n even, as claimed. Finally, we note that the recursion (298) entails that if (301) holds at τ_i, then (300) holds formally for all τ.

Assume now that to some order N the $s_1(\tau),\dots s_N(\tau)$ have been computed by the recursion (298) with initial data (299), (301). Then

$$S_p^{(N)}(\tau):=\frac{\exp\{-ip\int_{\tau_0}^{\tau}ds\,\omega_2(s)\}}{\sqrt{2p\omega_2(\tau)}}\Big\{1+\sum_{n=1}^{N}(ip)^{-n}s_n(\tau)\Big\}\,, \tag{303}$$

is unambigously defined. It enters our work horse Lemma:

Lemma 5.4.1. *For some $N>1$ let $S_p^{(N)}(\tau)$ be as in (303). Then, the differential equation $[\partial_\tau^2+\omega_p(\tau)^2]S_p(\tau)=0$ admits an exact (though implicitly N-dependent), Wronskian normalized ($\partial_\tau S_p(\tau)S_p(\tau)^*-S_p(\tau)\partial_\tau S_p(\tau)^*=-i$), complex solution S_p, such that*

$$\begin{aligned} S_p(\tau) &= S_p^{(N)}(\tau)\big[1+O(p^{-N})\big] \\ \partial_\tau S_p(\tau) &= \partial_\tau S_p^{(N)}(\tau)\big[1+O(p^{-N})\big]\,, \end{aligned} \tag{304}$$

uniformly in $\tau\in[\tau_i,\tau_f]$ as $p\to\infty$.

Here and below the O remainders refer to the supremum of the modulus of the function $f\in C[\tau_i,\tau_f]$ estimated, i.e. $f(\tau)=O(p^{-N})$ means $\|f\|)_{\sup}=O(p^{-N})$. The existence of such estimates for an order dependent function in terms of partial sums will below be indicated by the "$\asymp_N$" relation for the infinite series. For example, Lemma 5.4.1 amounts to the "$\asymp_N$" equality of both sides in (297). The asymptotic expansion of a fixed (N-independent) function will be denoted by "$\asymp$".

Proof.

To establish the existence and asymptotics of the solution S_p, we substitute

$$S_p(\tau)=S_p^{(N)}(\tau)\cdot R_p(\tau)\,, \tag{305}$$

into the differential equation $[\partial_\tau^2 + \omega_p(\tau)^2]S_p(\tau) = 0$ to obtain

$$\partial_\tau^2 R_p + 2\frac{\partial_\tau S_p^{(N)}}{S_p^{(N)}}\,\partial_\tau R_p + F(\tau,p)R_p = 0\,, \quad \text{with}$$

$$F_p(\tau) := \frac{\partial_\tau^2 S_p^{(N)} + \omega_p(\tau)^2 S_p^{(N)}}{S_p^{(N)}}\,. \tag{306}$$

It is readily verified from the recursion relations (298) that $\partial_\tau^2 S_p^{(N)} + \omega_p(\tau)^2 S_p^{(N)} = O(p^{-N-1/2})$, while $S_p^{(N)} = O(p^{-1/2})$, uniformly in $\tau \in [\tau_i, \tau_f]$ as $p \to \infty$. This entails

$$F_p(\tau) = O(p^{-N}) \quad \text{uniformly in } \tau \in [\tau_i, \tau_f] \text{ as } p \to \infty\,. \tag{307}$$

Defining the kernel

$$K_p(\tau,\tau') := \int_{\tau'}^{\tau} S_p^{(N)}(\tau')^2\, S_p^{(N)}(\tau'')^{-2} d\tau''\,, \tag{308}$$

it is easy to see that a function $R_p(\tau)$ satisfying the integral equation

$$R_p(\tau) = 1 + r_p - \int_{\tau_i}^{\tau} K_p(\tau,\tau')F_p(\tau')R_p(\tau')d\tau'\,, \tag{309}$$

solves (306). Here $r_p \in \mathbb{R}$ is a constant, satisfying $R_p(\tau_i) = 1 + r_p$, that will be determined later on. Further, $K_p = O(1)$ uniformly on $[\tau_i, \tau_f]^2$; so for sufficiently large p it follows from (307) that the map

$$u(\tau) \mapsto 1 + r_p - \int_{\tau_i}^{\tau} K_p(\tau,\tau')F_p(\tau')u(\tau')d\tau'\,, \tag{310}$$

is a contraction on the Banach space $\big(C([\tau_i,\tau_f],\mathbb{C}), \|\cdot\|_{\sup}\big)$; c.f (274). Hence (309) has a unique solution by the Banach Fixed Point theorem. Moreover, $R_p(\tau)$ is differentiable, with

$$\partial_\tau R_p(\tau) \;=\; -\int_{\tau_i}^{\tau} S_p^{(N)}(\tau')^2\, S_p^{(N)}(\tau)^{-2} F(\tau',p)R_p(\tau')d\tau'\,. \tag{311}$$

We now determine the constant r_p by imposing the Wronskian condition (303). Since $S_p(\tau) = S_p^{(N)}(\tau)\cdot R_p(\tau)$ solves $[\partial_\tau^2 + \omega_p(\tau)^2]S_p(\tau) = 0$, the Wronskian is conserved in time. Thus it is sufficient to demand that the normalization (303) holds for $\tau = \tau_i$. One has

$$\big(\partial_\tau S_p\, S_p^* - S_p\,\partial_\tau S_p^*\big)(\tau_i)$$

$$
\begin{aligned}
&= \big[\partial_\tau S_p^{(N)}\, S_p^{(N)\,*} - S_p^{(N)}\,\partial_\tau S_p^{(N)\,*}\big](\tau_i)\cdot R_p(\tau_i)R_p(\tau_i)^* \\
&+ S_p^{(N)}(\tau_i)S_p^{(N)\,*}(\tau_i)\cdot\big[\partial_\tau R_p\, R_p^* - R_p\,\partial_\tau R_p^*\big](\tau_i) \\
&= (1+r_p)^2\,\big[\partial_\tau S_p^{(N)}\, S_p^{(N)\,*} - S_p^{(N)}\,\partial_\tau S_p^{(N)\,*}\big](\tau_i)\,. \qquad (312)
\end{aligned}
$$

The expression $[\partial_\tau S_p^{(N)}\, S_p^{(N)\,*} - S_p^{(N)}\,\partial_\tau S_p^{(N)\,*}](\tau_i)$ may be expanded in powers of p^{-2} as before. Although this is a finite sum, in order to make contact to the formal Wronskian normalization (300), (301), it is convenient to regard the sum as being infinite, with the understanding that $s_n \equiv 0$ for $n > N$. With this understanding

$$
\begin{aligned}
&\big[\partial_\tau S_p^{(N)}\, S_p^{(N)\,*} - S_p^{(N)}\,\partial_\tau S_p^{(N)\,*}\big](\tau_i) \\
&= -i + i\sum_{k\geq 1}(-)^{k+1}p^{-2k}\Big\{\sum_{m,\,n\geq 0,\,m+n=k}(s_{2n}s_{2m})(\tau_i) - \sum_{m,\,n\geq 0,\,2m+n=2k-1}(\omega_2^{-1}s_n'\,s_{2m})(\tau_i)\Big\} \\
&=: i(-1+\delta_p) \qquad (313)
\end{aligned}
$$

Then

$$
\big(\partial_\tau S_p\, S_p^* - S_p\,\partial_\tau S_p^*\big)(\tau_i) \;=\; -i + i\big[(1+r_p)^2(-1+\delta_p)+1\big]\,, \qquad (314)
$$

and the appropriate normalization is thus ensured by choosing r_p such that the term in square brackets vanishes. In order to determine the large p behavior of r_p, that of δ_p is needed. To this end we decompose the sum in (313) as

$$
\begin{aligned}
\delta_p &= \sum_{k\geq 1}^{\lfloor N/2\rfloor}(-)^{k+1}p^{-2k}\Big\{\sum_{m,\,n\geq 0,\,m+n=k}(s_{2n}s_{2m})(\tau_i) - \sum_{m,\,n\geq 0,\,2m+n=2k-1}(\omega_2^{-1}s_n'\,s_{2m})(\tau_i)\Big\} \\
&+ \sum_{k>\lfloor N/2\rfloor}(-)^{k+1}p^{-2k}\Big\{\sum_{m,\,n\geq 0,\,m+n=k}(s_{2n}s_{2m})(\tau_i) - \sum_{m,\,n\geq 0,\,2m+n=2k-1}(\omega_2^{-1}s_n'\,s_{2m})(\tau_i)\Big\}\,, \qquad (315)
\end{aligned}
$$

again with the understanding that $s_n \equiv 0, n > N$. The highest index of s_n appearing in the first sum is $s_{2\lfloor N/2\rfloor}$, leaving it unaffected by setting $s_n \equiv 0$ for $n > N$. Hence the first sum in (315) vanishes as before, while the remainder contains only a finite number of nonzero terms

$$
\delta_p = \sum_{k>\lfloor N/2\rfloor}(-)^{k+1}p^{-2k}\Big\{\sum_{m,\,n\geq 0,\,m+n=k}(s_{2n}s_{2m})(\tau_i) - \sum_{m,\,n\geq 0,\,2m+n=2k-1}(\omega_2^{-1}s_n'\,s_{2m})(\tau_i)\Big\}\,.
$$

(316)

In general this remainder is nonzero, but it manifestly obeys $\delta_p = O(p^{-N-1})$. Solving $(1 + r_p)^2(-1 + \delta_p) + 1 = 0$ for r_p and choosing the positive square root one has

$$r_p \;=\; -1 + \sqrt{1 + \frac{\delta_p}{1 - \delta_p}} = O(p^{-N-1})\,, \tag{317}$$

on account of $\delta_p = O(p^{-N-1})$.

Having established the normalization (300) we now proceed to establish (304). It follows from (307), (309), and (317) that

$$R_p(\tau) = 1 + O(p^{-N}) \quad \text{uniformly in } \tau \in [\tau_i, \tau_f] \text{ as } p \to \infty\,, \tag{318}$$

proving the existence of an exact $S_p(\tau)$ such that $S_p(\tau) = S_p^{(N)}(\tau)[1 + O(p^{-N})]$. On account of the same estimates (311) entails $\partial_\tau R_p(\tau) = O(p^{-N})$, from which it follows that

$$\begin{aligned} \partial_\tau S_p(\tau) \;&=\; \partial_\tau S_p^{(N)}(\tau)\left[R_p(\tau) + \frac{S_p^{(N)}(\tau)}{\partial_\tau S_p^{(N)}(\tau)}\,\partial_\tau R_p(\tau)\right] \\ &=\; \partial_\tau S_p^{(N)}(\tau)\big[1 + O(p^{-N})\big]\,. \end{aligned} \tag{319}$$

This completes the proof.

□

Remarks:

(i) Using the results of [68] one can show that $s_n, n = 1, \ldots N$, coincide with the ones induced by the adiabatic iteration for sufficiently large order upon expansion in $1/p$. The recursion (298) with initial data (299), (301) in this sense replaces the adiabatic iteration.

(ii) A WKB ansatz of the form (297) has been analyzed in [76] recently, and was shown to be Borel summable under additional assumptions. These assumptions are typically not satisfied in massive theories, but may be attainable in massless ones. Our Lemma gives a weaker result which however directly applies to both situations.

(iii) The Lemma implies analogous asymptotic expansions for products of $S_p(\tau)$'s, both at identical and at distinct times. We prepare below the requisite notation for the two-point function (320), the modulus square (322), and the commutator function (323).

For the two-point function's Fourier kernel the Lemma implies

$$S_p(\tau)S_p(\tau')^* \asymp_N \frac{\exp\left\{-ip\int_{\tau'}^{\tau}ds\,\omega_2(s)\right\}}{2p\sqrt{\omega_2(\tau)\omega_2(\tau')}}\sum_{n\geq 0}V_n(\tau,\tau')(ip)^{-n}$$

$$V_n(\tau,\tau') = \sum_{j=0}^{n}(-)^{n-j}s_j(\tau)s_{n-j}(\tau')\,,\quad n\geq 0\,. \tag{320}$$

To low orders $V_0 = 1, V_1(\tau,\tau') = s_1(\tau) - s_1(\tau')$, $V_2(\tau,\tau') = s_2(\tau) - s_1(\tau)s_1(\tau') + s_2(\tau')$, etc.. Generally, the coefficients obey

$$V_{2j}(\tau,\tau') = V_{2j}(\tau',\tau)\,,\quad V_{2j+1}(\tau,\tau') = -V_{2j+1}(\tau',\tau)\,,\quad j\geq 0\,. \tag{321}$$

They can be evaluated from (298), (299), (301) recursively to any desired order and are increasingly nonlocal; see (348) for $n = 1, 2, 3$.

For the modulus square this results in an asymptotic expansion in odd inverse powers of p,

$$|S_p(\tau)|^2 \asymp_N \frac{1}{2\omega_2(\tau)}\sum_{n\geq 0}(-)^n V_{2n}(\tau,\tau)\frac{1}{p^{2n+1}}\,. \tag{322}$$

When used in (296) this establishes the existence of WKB type asymptotic expansions.

For the commutator function the Lemma implies

$$\begin{aligned}
\Delta_p(\tau,\tau') &= \Lambda_p^+(\tau,\tau')\sin\left(p\int_{\tau'}^{\tau}ds\,\omega_2(s)\right) + \Lambda_p^-(\tau,\tau')\cos\left(p\int_{\tau'}^{\tau}ds\,\omega_2(s)\right)\,.\\
\Lambda_p^+(\tau,\tau') &\asymp_N \frac{1}{\sqrt{\omega_2(\tau)\omega_2(\tau')}}\sum_{j\geq 0}p^{-2j-1}(-)^j V_{2j}(\tau,\tau')\,,\\
\Lambda_p^-(\tau,\tau') &\asymp_N \frac{1}{\sqrt{\omega_2(\tau)\omega_2(\tau')}}\sum_{j\geq 0}p^{-2j-2}(-)^j V_{2j+1}(\tau,\tau')\,.
\end{aligned} \tag{323}$$

5.4.2 Generalized resolvent expansion

As highlighted in (296), a Wronskian normalized solution of the basic wave equation is fully determined by its modulus square. By (322) we know the form of the modulus square's asymptotic expansion. The coefficients $V_{2n}(\tau,\tau)$ are in principle determined by the basic recursion (298). Since at each order an additional integration enters, one would expect these coefficients to be highly nonlocal in time. Remarkably, this is not the case: the $V_{2n}(\tau,\tau)$

turn out to be local differential polynomials in the frequency functions $\omega_0(\tau)^2, \omega_2(\tau)^2$ of the differential operator $\partial_\tau^2 + \omega_0(\tau)^2 + p^2\omega_2(\tau)^2$.

The main ingredient in the derivation is the Gelfand-Dickey equation. Using only the basic differential equation and the Wronskian normalization (193) one finds $|S_p(\tau)|^2$ to satisfy the (nonlinear form of the) Gelfand-Dickey equation

$$2|S_p|^2\partial_\tau^2|S_p|^2 - \big(\partial_\tau|S_p|^2\big)^2 + 4\omega_p^2|S_p|^4 = 1\,. \tag{324}$$

In view of the expected relation to (297) it is convenient to set

$$|S_p(\tau)|^2 =: iG_{ip}(\tau)\,. \tag{325}$$

Then

$$\begin{aligned} &2G_z\partial_\tau^2 G_z - (\partial_\tau G_z)^2 + 4[\omega_0^2 - z^2\omega_2^2]G_z^2 = -1\,,\\ &\partial_\tau^3 G_z + 4[\omega_0^2 - z^2\omega_2^2]\partial_\tau G_z + 2\partial_\tau[\omega_0^2 - z^2\omega_2^2]G_z = 0\,. \end{aligned} \tag{326}$$

Here the second, linear version of the Gelfand-Dickey equation follows by differentiating the nonlinear form. For $\omega_2^2 = 1$ and $\omega_0^2 = v$ the same equations govern the diagonal of the resolvent kernel of the differential operator $\partial_\tau^2 + v$, with $z^2 = -p^2$ playing the role of the resolvent parameter [29]. The diagonal of the resolvent kernel is known to admit an asymptotic expansion in inverse powers of z, whose coefficients coincide with the heat kernel coefficients on general grounds, see e.g. [4]. The generalization to $[\partial_\tau^2+\omega_0(\tau)^2]S = z^2\omega_2(\tau)^2 S$, with non-constant $\omega_2(\tau)^2$ can be treated as follows.

Inserting the ansatz

$$G_z(\tau) = \sum_{n\geq 0}\frac{G_n(\tau)}{2\omega_2}z^{-2n-1}\,,\quad G_0 = 1\,, \tag{327}$$

into the nonlinear Gelfand-Dickey equation results in the recursion

$$G_n = \sum_{k,l\geq 0, k+l=n-1}\Big\{\frac{1}{4}\frac{G_k}{\omega_2}\partial_\tau^2\Big(\frac{G_l}{\omega_2}\Big) - \frac{1}{8}\partial_\tau\Big(\frac{G_k}{\omega_2}\Big)\partial_\tau\Big(\frac{G_l}{\omega_2}\Big) + \frac{1}{2}\frac{\omega_0^2}{\omega_2^2}G_kG_l\Big\} - \frac{1}{2}\sum_{k,l\geq 1, k+l=n}G_kG_l. \tag{328}$$

This expresses G_n in terms of $G_{n-1}, \ldots, G_1$, and involves only differentiations. It follows that all G_n are differential polynomials in $v := \omega_0^2, w := \omega_2^2$. Denoting ∂_τ differentiations momentarily by a "$'$" one finds:

$$\begin{aligned} G_1 &= \frac{v}{2w} + \frac{5}{32}\frac{w'^2}{w^3} - \frac{1}{8}\frac{w''}{w^2}\,, \\ G_2 &= \frac{3}{8w^2}\Big(v^2 + \frac{1}{3}v''\Big) - \frac{5}{16w^3}\Big(vw'' + v'w' - v\frac{7w'^2}{4w}\Big) \\ &+ \frac{1}{32w^3}\Big(-w^{(4)} + \frac{21w''^2}{4w} + \frac{7w^{(3)}w'}{w} - \frac{231w'^2w''}{8w^2} + \frac{1155w'^4}{64w^3}\Big)\,. \end{aligned} \tag{329}$$

The recursion (328) is easily programmed in `Mathematica` and produces the G_n to reasonably high orders. The G_n can be seen as generalized heat kernel coefficients. For $\omega_2 = 1$, $v = \omega_0^2$ plays the role of the potential and (329) reproduces the well-known expressions [4] (up to overall normalizations). In the massless case $v = \omega_0^2 = 0$, and only the purely w dependent parts of the G_n remain. From the viewpoint of the initial expansion (297), (298) the concise differential polynomials (329) are surprising: $G_n = V_{2n}(\tau, \tau)$ must hold by construction, but would seem to suggest highly nonlocal coefficients. At low orders one can see the cancellation of the nonlocal terms directly. For example, the $n = 2$ recursion (298) integrates to $s_2 = s_1^2/2 + \partial_\tau s_1/(2\omega_2)$. Hence $G_1 = 2s_2 - s_1^2 = \partial_\tau s_1/\omega_2$, which is indeed local.

One can also relate the G_n's more directly to the standard heat kernel coefficients. To this end, we transform the basic differential equation (193) into conformal time as in (196), but for generic frequency functions: $\partial_\eta = \omega_2(\tau)^{-1}\partial_\tau$, $\chi_p(\tau) = \omega_2(\tau)^{1/2} S_p(\tau)|_{\tau=\tau(\eta)}$. This replaces the differential operator $\partial_\tau^2 + \omega_0(\tau)^2 + p^2\omega_2(\tau)^2$ by $\partial_\eta^2 + 2E_1(\eta) + p^2$, with $E_1(\eta) = G_1(\tau(\eta))$, the image of G_1 in (329). The coefficient of p^2 is now unity and $2E_1(\eta)$ plays the role of the potential. Inserting the η-version of the ansatz (327) into the linear Gelfand-Dickey equation results in the one-step differential recursion

$$\partial_\eta E_{n+1} = \partial_\eta E_1 E_n + 2E_1\partial_\eta E_n + \frac{1}{4}\partial_\eta^3 E_n\,, \quad n \geq 1\,. \tag{330}$$

This defines (up to a conventional normalization) the standard heat kernel coefficients with potential $2E_1$. Undoing the transformation one has

$$G_n = E_n\big|_{E_1 \mapsto G_1, \partial_\eta \mapsto \omega_2(\tau)^{-1}\partial_\tau}\,. \tag{331}$$

For example, for $n = 2$ this gives

$$G_2 = \frac{3}{2}G_1^2 + \frac{1}{4\omega_2}\partial_\tau\Big(\frac{\partial_\tau G_1}{\omega_2}\Big)\,, \tag{332}$$

which is indeed satisfied by (329). Generally, the agreement of (328) with (331) provides a welcome check.

An analogous interplay exists for the asymptotics of the phase as induced by the basic expansion (297) and the resolvent expansion (327), respectively. Starting from the basic expansion (297) the phase is determined by $\tan(\arg S_p(\tau)) = \Im S_p(\tau)/\Re S_p(\tau)$. One finds

$$\begin{aligned}
&\tan\big(\arg S_p(\tau)\big) = -\frac{\mathcal{S}_p^-(\tau)\mathbf{C}_p + \mathcal{S}_p^+(\tau)\mathbf{S}_p}{\mathcal{S}_p^+(\tau)\mathbf{C}_p - \mathcal{S}_p^-(\tau)\mathbf{S}_p}\,,\\
&\mathbf{S}_p = \sin\Big(p\int_{\tau'}^{\tau} ds\,\omega_2(s)\Big)\,, \quad \mathbf{C}_p = \cos\Big(p\int_{\tau'}^{\tau} ds\,\omega_2(s)\Big)\,.
\end{aligned} \tag{333}$$

with

$$\begin{aligned}
\mathcal{S}_p^+(\tau) &\asymp_N \frac{1}{\sqrt{2p\omega_2(\tau)}}\sum_{j\geq 0}(-)^j s_{2j}(\tau)p^{-2j}\,,\\
\mathcal{S}_p^-(\tau) &\asymp_N \frac{1}{\sqrt{2p\omega_2(\tau)}}\sum_{j\geq 0}(-)^j s_{2j+1}(\tau)p^{-2j-1}\,,
\end{aligned} \tag{334}$$

To low orders

$$\begin{aligned}
&\tan\big(\arg S_p(\tau)\big) \asymp_N -\frac{\mathbf{S}_p}{\mathbf{C}_p} - \frac{1}{p}s_1(\tau)\frac{1}{\mathbf{C}_p^2} - \frac{1}{p^2}s_1(\tau)^2\frac{\mathbf{S}_p}{\mathbf{C}_p^3} - \frac{1}{p^3}s_1(\tau)^3\frac{\mathbf{S}_p^2}{\mathbf{C}_p^4}\\
&-\frac{1}{p^3}(s_1s_2 - s_3)(\tau)\frac{1}{\mathbf{C}_p^2} + O\Big(\frac{1}{p^4}\Big)\,.
\end{aligned} \tag{335}$$

Writing $s_1s_2 - s_3 = s_1^3/3 - u_3$, the ratios of trigonometric functions are just the derivatives of the tan function; so (335) is equivalent to

$$\begin{aligned}
\arg S_p(\tau) \;&\asymp_N\; -p\int_{\tau_0}^{\tau} ds\,\omega_2(s) - \frac{s_1(\tau)}{p} + \frac{u_3(\tau)}{p^3} + O\Big(\frac{1}{p^5}\Big)\,,\\
u_3(\tau) \;&=\; \frac{\partial_\tau G_1}{4\omega_2} + \frac{1}{2}\int_{\tau_0}^{\tau} ds\,\omega_2(s)G_1(s)^2\,, \quad G_1(\tau) = \frac{\partial_\tau s_1}{\omega_2}\,,
\end{aligned} \tag{336}$$

where the explicit form of u_3 follows from the recursion (298). Proceeding along these lines, it is not immediate that at higher orders no oscillatory terms will occur in the phase itself

and that the coefficients will be single integrals of local quantities.

This is, however, the case and can be seen from the alternative realization of the phase entailed by (296) and (325)

$$\arg S_p(\tau) = -\frac{1}{2}\int_{\tau_0}^{\tau} ds\, \frac{1}{iG_{ip}(s)}\,. \tag{337}$$

Here the expansion (327) can be used. It follows that $\arg S_p(\tau)$ admits an asymptotic expansion in odd inverse powers of p whose coefficients are *single* integrals of polynomials in the G_n. To low orders

$$\frac{1}{iG_{ip}(\tau)} \asymp_N 2\omega_2(\tau)p\Big\{1 + \frac{G_1(\tau)}{p^2} + \frac{(G_1^2 - G_2)(\tau)}{p^4} + O\Big(\frac{1}{p^6}\Big)\Big\}\,. \tag{338}$$

The equivalence to (336) is ensured by (332).

5.4.3 Induced asymptotic expansion of SLE

Using the formulas from Theorem 5.2.2 and (323) all SLE related quantities have induced asymptotic expansions in inverse powers of p at some finite order $N > 1$. The order can be increased arbitrarily, but in general the exact reference solution in Lemma 5.4.1 needs to be changed in order to do so. Here we show that the (unique, N-independent) SLE solution is asymptotic $\asymp_N$ to the previously constructed series for *all* N. In particular, the asymptotic expansion is independent of the window function f.

Theorem 5.4.2. The modulus-square of the SLE solution admits an asymptotic expansion in odd inverse powers of p, whose coefficients are independent of the window function f and are given by generalized heat kernel coefficients. Specifically

$$|T_p^{\mathrm{SLE}}(\tau)|^2 \asymp \frac{1}{2p\omega_2(\tau)}\left\{1 + \sum_{n\geq 1}\frac{(-)^n}{p^{2n}}G_n(\tau)\right\}\,, \tag{339}$$

where the G_n are determined recursively by (328). The phase has an asymptotic expansion obtained from

$$\arg T_p^{\mathrm{SLE}}(\tau) \asymp -p\int_{\tau_0}^{\tau} ds\, \omega_2(s)\left\{1 + \sum_{n\geq 1}\frac{(-)^n}{p^{2n}}G_n(\tau)\right\}^{-1}\,. \tag{340}$$

The massless limits are regular and have coefficients $G_n|_{\omega_0^2=0}$.

Proof.

We mostly need to show that $|T_p^{\rm SLE}(\tau)|^2$ admits an asymptotic expansion of the form (339) with some coefficients $\tilde{G}_n(\tau)$. Since the SLE solution is a Wronskian normalized solution of the basic wave equation, its modulus square solves the nonlinear Gelfand-Dickey equation (324). The coefficients $\tilde{G}_n(\tau)$ therefore also have to obey the recursion (328). It then suffices to check by direct computation that $\tilde{G}_0 = 1$. The latter will be done separately following the proof. Since $\tilde{G}_0 = 1$ determines all other coefficients, it follows that $\tilde{G}_n = G_n$, for all $n \in \mathbb{N}$. The relation (340) between phase and modulus holds on account of the Wronskian normalization.

In order to show that $|T_p^{\rm SLE}(\tau)|^2$ has an asymptotic expansion in odd inverse powers of p, we use the realization as $J_p(\tau)/(2\mathcal{E}_p^{\rm SLE})$ from (253). The integrands of $J_p(\tau)$ and $(\mathcal{E}_p^{\rm SLE})^2$ are built from $\Delta_p(\tau,\tau_0)$, $\partial_\tau\Delta_p(\tau,\tau_0)$, $\partial_\tau\partial_{\tau_0}\Delta_p(\tau,\tau_0)$. For these we prepare

$$\begin{aligned}
\Delta_p(\tau,\tau') &= \Lambda_p^+(\tau,\tau')\mathbf{S}_p + \Lambda_p^-(\tau,\tau')\mathbf{C}_p\,,\\
\partial_\tau\Delta_p(\tau,\tau') &= \cap_p^+(\tau,\tau')\mathbf{S}_p + \cap_p^-(\tau,\tau')\mathbf{C}_p\,,\\
\partial_\tau\partial_{\tau'}\Delta_p(\tau,\tau') &= \sqcap_p^+(\tau,\tau')\mathbf{S}_p + \sqcap_p^-(\tau,\tau')\mathbf{C}_p\,,
\end{aligned} \tag{341}$$

with $\mathbf{S}_p$, $\mathbf{C}_p$ as defined in (333), and

$$\begin{aligned}
\cap_p^\pm(\tau,\tau') &= \partial_\tau\Lambda^\pm(\tau,\tau') \mp p\omega_2(\tau)\Lambda^\mp(\tau,\tau')\,,\\
\sqcap_p^\pm(\tau,\tau') &= \partial_{\tau'}\partial_\tau\Lambda_p^\pm(\tau,\tau') \pm p[\partial_\tau\Lambda^\mp(\tau,\tau')\omega_2(\tau') - \partial_{\tau'}\Lambda^\mp(\tau,\tau')\omega_2(\tau)]\\
&+ p^2\omega_2(\tau)\omega_2(\tau')\Lambda^\pm(\tau,\tau')\,.
\end{aligned} \tag{342}$$

Note that $\Lambda_p^\pm(\tau,\tau') = \pm\Lambda_p^\pm(\tau',\tau)$, $\sqcap_p^\pm(\tau,\tau') = \pm\sqcap_p^\pm(\tau',\tau)$, while $\cap_p^\pm(\tau,\tau')$ has no manifest symmetry. The normalization of the commutator function implies, however, $\cap_p^-(\tau,\tau) = 1$. The definitions in combination with (323) imply that $\Lambda_p^+, \cap_p^+, \sqcap_p^+$ have an asymptotic $\asymp_N$ expansion in odd inverse powers of p, while $\Lambda_p^-, \cap_p^-, \sqcap_p^-$ have an asymptotic $\asymp_N$ expansion in even inverse powers of p. Crucially, while the fiducial solutions S_N provided by Lemma 5.4.1 are implicitly N-dependent, Theorem 5.2.1 ensures that the induced expansion of $|T_p^{\rm SLE}(\tau)|^2$

is independent thereof. Schematically, $|T_p^{\mathrm{SLE}}[S_N]|^2$ is the same for all N, which allows one to take N arbitrarily large.

Next we use (341) to evaluate the integrands of $J_p(\tau')$ from (244) and $(\mathcal{E}_p^{\mathrm{SLE}})^2$ from (252). In a first step we merely insert (341) and replace all powers of oscillatory terms by linear ones using

$$\mathbf{S}_p^2 = \frac{1}{2}(1 - \mathbf{C}_{2p})\,, \quad \mathbf{C}_p^2 = \frac{1}{2}(1 + \mathbf{C}_{2p})\,, \quad \mathbf{S}_p\mathbf{C}_p = \frac{1}{2}\mathbf{S}_{2p}\,. \tag{343}$$

This gives

$$\begin{aligned}
&(\partial_\tau \Delta_p(\tau,\tau'))^2 + \omega_p(\tau)^2 \Delta_p(\tau,\tau')^2 \\
&= \frac{1}{2}\Big[\cap_p^+(\tau,\tau')^2 + \cap_p^-(\tau,\tau')^2 + \omega_p(\tau)^2\big(\Lambda_p^+(\tau,\tau')^2 + \Lambda_p^-(\tau,\tau')^2\big)\Big] \\
&-\frac{1}{2}\Big[\cap_p^+(\tau,\tau')^2 - \cap_p^-(\tau,\tau')^2 + \omega_p(\tau)^2\big(\Lambda_p^+(\tau,\tau')^2 - \Lambda_p^-(\tau,\tau')^2\big)\Big]\mathbf{C}_{2p} \\
&+\Big[(\cap_p^+\cap_p^-)(\tau,\tau') + \omega_p(\tau)^2(\Lambda_p^+\Lambda_p^-)(\tau,\tau')\Big]\mathbf{S}_{2p}\,.
\end{aligned} \tag{344}$$

The integrand of $(\mathcal{E}_p^{\mathrm{SLE}})^2$ is of course symmetrized in τ,τ'; for brevity's sake we use the non-symmetric version

$$\begin{aligned}
&\big(\partial_\tau\partial_{\tau'}\Delta_p(\tau,\tau')\big)^2 + 2\omega_p(\tau')^2\big(\partial_\tau\Delta_p(\tau,\tau')\big)^2 + \omega_p(\tau)^2\omega_p(\tau')^2\Delta_p(\tau,\tau')^2 \\
&= \frac{1}{2}\Big[\sqcap_p^+(\tau,\tau')^2 + \sqcap_p^-(\tau,\tau')^2 + 2\omega_p(\tau')^2\big(\cap_p^+(\tau,\tau')^2 + \cap_p^-(\tau,\tau')^2\big) \\
&+\omega_p(\tau)^2\omega_p(\tau')^2\big(\Lambda_p^+(\tau,\tau')^2 + \Lambda_p^-(\tau,\tau')^2\big)\Big] \\
&-\frac{1}{2}\Big[\sqcap_p^+(\tau,\tau')^2 - \sqcap_p^-(\tau,\tau')^2 + 2\omega_p(\tau')^2\big(\cap_p^+(\tau,\tau')^2 - \cap_p^-(\tau,\tau')^2\big) \\
&+\omega_p(\tau)^2\omega_p(\tau')^2\big(\Lambda_p^+(\tau,\tau')^2 - \Lambda_p^-(\tau,\tau')^2\big)\Big]\mathbf{C}_{2p} \\
&+\Big[(\sqcap_p^+\sqcap^-)(\tau,\tau') + 2\omega_p(\tau')^2(\cap_p^+\cap_p^-)(\tau,\tau') \\
&+\omega_p(\tau)^2\omega_p(\tau')^2(\Lambda_p^+\Lambda_p^-)(\tau,\tau')\Big]\mathbf{S}_{2p}\,.
\end{aligned} \tag{345}$$

The coefficients of the oscillatory terms have asymptotic expansions in inverse powers of p which are uniform the both variables. Focussing on the integration variable we write $A_p(\tau)$ for such a coefficient. For smooth ω_0, ω_2 also A_p will be smooth in τ. By repeated use of the

integrations-by-parts identities

$$\mathbf{S}_{2p} = -\frac{1}{2p\omega_2(\tau)}\partial_\tau \mathbf{C}_{2p}\,, \quad \mathbf{C}_{2p} = \frac{1}{2p\omega_2(\tau)}\partial_\tau \mathbf{S}_{2p}\,,$$
$$\int d\tau f(\tau)^2 A_p(\tau)\mathbf{S}_{2p} = \frac{1}{2p}\int d\tau \partial_\tau \left(\frac{f(\tau)^2 A_p(\tau)}{\omega_2(\tau)}\right)\mathbf{C}_{2p}\,,$$
$$\int d\tau f(\tau)^2 A_p(\tau)\mathbf{C}_{2p} = -\frac{1}{2p}\int d\tau \partial_\tau \left(\frac{f(\tau)^2 A_p(\tau)}{\omega_2(\tau)}\right)\mathbf{S}_{2p}\,, \tag{346}$$

the oscillatory terms can therefore be made subleading at any desired order of the asymptotic expansion.

It follows that at any order the asymptotic expansion of $J_p(\tau')$ and $(\mathcal{E}_p^{\mathrm{SLE}})^2$ is generated by the non-oscillatory terms in (344), (345). By inspection of the orders induced by (323) and (342) one sees that the non-oscillatory term in (344) has an expansion in even inverse powers of p, starting with a $O(p^0)$ term. Similarly p^{-2} times the non-oscillatory term in (345) has an expansion in even inverse powers of p, starting with a $O(p^0)$ term. Hence $J_p(\tau')$ has an asymptotic expansion in even inverse powers of p, starting with an $O(p^0)$ term. The square root of the non-oscillatory term in (345) governs the expansion of $p^{-1}\mathcal{E}_p^{\mathrm{SLE}}$, which therefore likewise has an asymptotic expansion in even inverse powers of p, starting with a $O(p^0)$ term. Together, $J_p(\tau)/(2\mathcal{E}_p^{\mathrm{SLE}})$ admits a asymptotic expansion in odd inverse powers of p, as claimed. Augmented by the explicit computation of the leading order, this implies the result. □

Remarks:

(i) The exponent in $\exp\{i \arg T_p^{\mathrm{SLE}}(\tau)\}$ can be re-expanded in powers of $1/p$ to obtain a simplified expansion of the form (297). Theorem 5.4.2 implies that $T_p^{\mathrm{SLE}}(\tau)$ has the property described in Lemma 5.4.1 for *any* $N > 1$. This replaces Olbermann's Lemma 4.5, where the adiabatic vacua of order N play a role analogous to our approximants $S_p^{(N)}(\tau)$ (though not necessarily with matched orders). The adiabatic vacua are however far less explicit: first, the adiabatic iteration produces more complicated formulas of which only the large p expansion is actually used. Second, the iterates are only well-defined for sufficiently large p, so for technical reasons they need to be extended in an ad-hoc manner to small momenta [68]. Third, the result then enters an integral equation whose iteration produces the required

exact solution, dubbed adiabatic vacuum of order N. The Lemma 5.4.1 short cuts these three steps. The ansatz (297) only processes the information relevant for large p and the iteration (298) is manifestly well-defined without modifications. In combination with (327), (328) this yields a practically usable expansion.

(ii) The simplified expansion from (i) for the product $T_p^{\mathrm{SLE}}(\tau)T_p^{\mathrm{SLE}}(\tau')^*$ can be viewed as the Fourier space version of the (state independent) Hadamard parametrix. The Hadamard parametrix also has a truncated version where only the solution of the recursion to some finite order is kept, see e.g. [61]. These truncations converge in a certain sense to the Hadamard parametrix proper, which in turn is a distributional solution of the wave equation in both arguments modulo a smooth piece. The fact that the inverse Fourier transform of the state independent WKB expansion has the form of the Hadamard parametrix was verified (in $d = 3$ and in conformal time) by an instructive if formal computation in [84]. In Olbermann's proof of the Hadamard property this step is rigorously supplied by appealing to a general result of Junker and Schrohe [56], describing the wave front set of adiabatic vacua of order N. Since our approximants have the same large p asymptotics as the adiabatic vacua (though not necessarily with matched orders) this step carries over. It may be worthwhile to attempt a direct, simplified proof, specific for SLE and including the massless case.

(iii) Assuming that the massless case can be treated along these lines the SLE would provide very relevant examples of *infrared finite Hadamard* states. Their relevance stems from the following *Proposal:* The primordial vacuum-like state (of a massless free QFT and the perturbation theory based on it) should be chosen to be an infrared finite Hadamard state and conceptually be associated with a pre-inflationary period of non-accelerated expansion. The rationale for this proposal is detailed in Section 5.5.

Direct verification of Theorem 5.4.2 to subleading order:

The proof of Theorem 5.4.2 hinges on the direct verification of the leading order asymptotics. Here we present an ab-initio evaluation of the $|T_p^{\mathrm{SLE}}(\tau|^2$ asymptotics to subleading order, starting from Eq. (253) and the asymptotics (323) of the commutator function. We prepare to subleading order

$$\Lambda_p^+(\tau,\tau') \;=\; \frac{1}{p}\tilde{V}_0(\tau,\tau') - \frac{1}{p^3}\tilde{V}_2(\tau,\tau') + O\Big(\frac{1}{p^5}\Big)\,,$$

$$
\begin{aligned}
\Lambda_p^-(\tau,\tau') &= \frac{1}{p^2}\tilde V_1(\tau,\tau') - \frac{1}{p^4}\tilde V_3(\tau,\tau') + O\Big(\frac{1}{p^6}\Big)\,,\\
\cap_p^+(\tau,\tau') &= \frac{1}{p}\big[\partial_\tau \tilde V_0(\tau,\tau') - \omega_2(\tau)\tilde V_1(\tau,\tau')\big] - \frac{1}{p^3}\big[\partial_\tau \tilde V_2(\tau,\tau') - \omega_2(\tau)\tilde V_3(\tau,\tau')\big] + O\Big(\frac{1}{p^5}\Big)\,,\\
\cap_p^-(\tau,\tau') &= \omega_2(\tau)\tilde V_0(\tau,\tau') + \frac{1}{p^2}\big[\partial_\tau \tilde V_1(\tau,\tau') - \omega_2(\tau)\tilde V_2(\tau,\tau')\big] + O\Big(\frac{1}{p^4}\Big)\,,\\
\sqcap_p^+(\tau,\tau') &= p\,\omega_2(\tau)\omega_2(\tau')\tilde V_0(\tau,\tau') + \frac{1}{p}\big[\partial_\tau\partial_{\tau'}\tilde V_0(\tau,\tau') + \partial_\tau \tilde V_1(\tau,\tau')\omega_2(\tau') - \partial_{\tau'}\tilde V_1(\tau,\tau')\omega_2(\tau)\\
&- \omega_2(\tau)\omega_2(\tau')\tilde V_2(\tau,\tau')\big] + O\Big(\frac{1}{p^3}\Big)\,,\\
\sqcap_p^-(\tau,\tau') &= -\partial_\tau \tilde V_0(\tau,\tau')\omega_2(\tau') + \partial_{\tau'}\tilde V_0(\tau,\tau')\omega_2(\tau) + \omega_2(\tau)\omega_2(\tau')\tilde V_1(\tau,\tau')\\
&+ \frac{1}{p^2}\big[\partial_\tau\partial_{\tau'}\tilde V_1(\tau,\tau') + \partial_\tau \tilde V_2(\tau,\tau')\omega_2(\tau') - \partial_{\tau'}\tilde V_2(\tau,\tau')\omega_2(\tau)\\
&- \omega_2(\tau)\omega_2(\tau')\tilde V_3(\tau,\tau')\big] + O\Big(\frac{1}{p^4}\Big)\,, \qquad (347)
\end{aligned}
$$

with

$$
\begin{aligned}
\tilde V_n(\tau,\tau') &:= \frac{V_n(\tau,\tau')}{\sqrt{\omega_2(\tau)\omega_2(\tau')}}\,, \quad V_0 = 1\,,\\
V_1(\tau,\tau') &= s_1(\tau) - s_1(\tau')\,, \quad V_2(\tau,\tau') = \frac{1}{2}V_1(\tau,\tau')^2 + \frac{1}{2}[G_1(\tau) + G_1(\tau')]\,,\\
V_3(\tau,\tau') &= \frac{1}{6}V_1(\tau,\tau')^3 + V_1(\tau,\tau')\big[G_1(\tau) + G_1(\tau')\big]\\
&+ \frac{\partial_\tau G_1(\tau)}{2\omega_2(\tau)} - \frac{\partial_{\tau'}G_1(\tau')}{2\omega_2(\tau')} - 2\int_{\tau'}^{\tau} ds\,\omega_2(s)G_1(s)^2\,. \qquad (348)
\end{aligned}
$$

As described in the proof, it suffices to focus on the non-oscillatory in (344), (345). Keeping up to subleading terms in (344) one finds

$$
\begin{aligned}
&(\partial_\tau \Delta_p(\tau,\tau'))^2 + \omega_p(\tau)^2\Delta_p(\tau,\tau')^2\\
&\asymp \omega_2(\tau)^2\tilde V_0(\tau,\tau')^2 + \frac{1}{p^2}\Big\{\frac{1}{2}(\partial_\tau \tilde V_0(\tau,\tau'))^2 + \frac{1}{2}\omega_0(\tau)^2\tilde V_0(\tau,\tau')^2\\
&+\omega_2(\tau)\big(\tilde V_0\partial_\tau\tilde V_1 - \partial_\tau\tilde V_0\tilde V_1\big)(\tau,\tau') + \omega_2(\tau)^2\big(\tilde V_1^2 - 2\tilde V_0\tilde V_2\big)(\tau,\tau')\Big\} + O\Big(\frac{1}{p^4}\Big). \qquad (349)
\end{aligned}
$$

Upon integration this gives

$$
J_p(\tau') \asymp \frac{\bar\omega_2}{2\omega_2(\tau')}\Big\{1 + \frac{1}{p^2}\Big[-G_1(\tau') + \frac{1}{2\bar\omega_2}\int d\tau\, f(\tau)^2\Big(\frac{\omega_0^2}{\omega_2} + \frac{1}{4}\frac{(\partial_\tau\omega_2)^2}{\omega_2^2}\Big)\Big] + O\Big(\frac{1}{p^4}\Big)\Big\}\,. \qquad (350)
$$

Here we used

$$\tilde{V}_1^2 - 2\tilde{V}_0\tilde{V}_2 = -\frac{G_1(\tau)+G_1(\tau')}{\omega_2(\tau)\omega_2(\tau')}\,,$$
$$\frac{1}{2}(\partial_\tau\tilde{V}_0)^2 + \frac{1}{2}\omega_0(\tau)^2\tilde{V}_0^2 = \frac{1}{2\omega_2(\tau)\omega_2(\tau')}\Big(\omega_0^2 + \frac{1}{4}\frac{(\partial_\tau\omega_2)^2}{\omega_2^2}\Big)\,,$$
$$2\omega_2^2 G_1 = \omega_0^2 + \frac{1}{4}\frac{(\partial_\tau\omega_2)^2}{\omega_2^2} - \frac{1}{2}\partial_\tau\Big(\frac{\partial_\tau\omega_2}{\omega_2}\Big)\,. \tag{351}$$

Similarly, keeping up to subleading terms in (345) one has

$$\begin{aligned}
&\big(\partial_\tau\partial_{\tau'}\Delta_p(\tau,\tau')\big)^2 + 2\omega_2(\tau')^2\big(\partial_\tau\Delta_p(\tau',\tau)\big)^2 + \omega_p(\tau)^2\omega_p(\tau')^2\Delta_p(\tau,\tau')^2\\
&\quad\asymp p^2\,2\omega_2(\tau)^2\omega_2(\tau')^2\tilde{V}_0^2 + \Big(\frac{1}{2}\omega_0(\tau)^2\omega_2(\tau')^2 + \frac{3}{2}\omega_0(\tau')^2\omega_2(\tau)^2\Big)\tilde{V}_0^2\\
&\quad+\omega_2(\tau)\omega_2(\tau')\tilde{V}_0\partial_\tau\partial_{\tau'}\tilde{V}_0 + \omega_2(\tau')^2(\partial_\tau\tilde{V}_0)^2 + \frac{1}{2}\big[\partial_\tau\tilde{V}_0\omega_2(\tau') - \partial_{\tau'}\tilde{V}_0\omega_2(\tau)\big]^2\\
+\quad&3\omega_2(\tau)\omega_2(\tau')^2\big(\tilde{V}_0\partial_\tau\tilde{V}_1 - \tilde{V}_1\partial_\tau\tilde{V}_0\big) - \omega_2(\tau)^2\omega_2(\tau')\big(\tilde{V}_0\partial_{\tau'}\tilde{V}_1 - \tilde{V}_1\partial_{\tau'}\tilde{V}_0\big)\\
+\quad&2\omega_2(\tau)^2\omega_2(\tau')^2\big(\tilde{V}_1^2 - 2\tilde{V}_0\tilde{V}_2\big) + O\Big(\frac{1}{p^2}\Big).
\end{aligned} \tag{352}$$

For the simplification we use (351) as well as

$$\tilde{V}_0\partial_\tau\tilde{V}_1 - \tilde{V}_1\partial_\tau\tilde{V}_0 = \frac{G_1(\tau)}{\omega_2(\tau')}\,,\quad \tilde{V}_0\partial_{\tau'}\tilde{V}_1 - \tilde{V}_1\partial_{\tau'}\tilde{V}_0 = -\frac{G_1(\tau')}{\omega_2(\tau)}\,, \tag{353}$$

For the $O(p^0)$ term in (352) this results in

$$\begin{aligned}
&\omega_2(\tau)\omega_2(\tau')\big(G_1(\tau) - G_1(\tau')\big) + \frac{1}{2}\frac{\omega_0(\tau)^2}{\omega_2(\tau)}\omega_2(\tau') + \frac{3}{2}\frac{\omega_0(\tau')^2}{\omega_2(\tau')}\omega_2(\tau)\\
&\quad+\frac{3}{8}\frac{(\partial_\tau\omega_2)^2}{\omega_2(\tau)^3}\omega_2(\tau') + \frac{1}{8}\frac{(\partial_{\tau'}\omega_2)^2}{\omega_2(\tau')^3}\omega_2(\tau)\,.
\end{aligned} \tag{354}$$

Finally,

$$(\mathcal{E}_p^{\mathrm{SLE}})^2 = \frac{p^2}{4}\bar{\omega}_2^2 + \frac{\bar{\omega}_2}{4}\int d\tau\, f(\tau)^2\Big(\frac{\omega_0^2}{\omega_2} + \frac{1}{4}\frac{(\partial_\tau\omega_2)^2}{\omega_2^3}\Big) + O\Big(\frac{1}{p^4}\Big)\,. \tag{355}$$

This results in

$$|T_p^{\mathrm{SLE}}(\tau)|^2 \asymp \frac{1}{2p\omega_2(\tau)}\left\{1 - \frac{1}{p^2}G_1(\tau) + O\Big(\frac{1}{p^4}\Big)\right\}\,. \tag{356}$$

The leading term confirms $\tilde{G}_0 = 1$ in the proof of Theorem 5.4.2. The subleading term

verifies the assertion at this order by an ab-initio computation.

As seen previously, the relation (340) between phase and modulus holds on account of the Wronskian normalization. However, it is not immediate how the expression (253) for $\tan(\arg T_p^{\mathrm{SLE}}(\tau))$ reproduces this simple answer. As a final check on the framework we verified the equivalence to subleading order by direct computation. Omitting the details, the result is

$$\tan\big(\arg T_p^{\mathrm{SLE}}(\tau)\big) = -\frac{\mathcal{E}_p^{\mathrm{SLE}}\Delta_p(\tau,\tau_0)}{J_p(\tau,\tau_0)} \asymp -\frac{\mathbf{S}_p}{\mathbf{C}_p} - \frac{s_1(\tau)}{p}\frac{1}{\mathbf{C}_p^2} + O\Big(\frac{1}{p^3}\Big)\,. \tag{357}$$

This agrees with (335) and hence (337), (338) to the order considered.

5.5 SLE as pre-inflationary vacua

One of the key empirical facts about the Cosmological Microwave Background (CMB) is its near scale invariance at large values of the multipole expansion. This feature, realized at $t = t_{\mathrm{decoupl}}$, is thought to be rooted in a similar behavior of the primordial power spectrum $P_\zeta(t_*, p)$ at the (cosmological) time $t_* \ll t_{\mathrm{decoupl}}$ when the seeds for structure formation are laid, for any of the relevant fluctuation variables ζ. In terms of the spatial Fourier momentum a behavior $P_\zeta(t_*, p) \sim |p|^{-2\nu}$ is needed, with ν close to $d/2$. Such a behavior is seemingly incompatible with the momentum dependence of the massless SLE modes. We show here that a qualitatively correct power spectrum arises at $t = t_*$, if a pre-inflationary period is followed by one of near-exponential expansion.

It must be stressed that general relativity *demands* a period of non-accelerated expansion following the Big Bang, i.e. for some interval $t \in (t_{\mathrm{sing}}, t_1]$. In particular, variants of the cosmological singularity theorems remain valid for generic inflationary spacetimes with positive cosmological constant [91]. For FL spacetimes a pre-inflationary phase with kinetic energy domination is preferred [38, 46]. As a consequence, the time-honored purely positive frequency Bunch-Davies vacuum, traditionally postulated at the beginning of the inflationary period cannot be physically realistic: the modes from the pre-inflationary period (whether themselves positive frequency or not close to the singularity) will generically *not* be positive

frequency at t_1. As a consequence the modes at $t = t_1$ can also not comply with deSitter invariance. This is because an admixture of positive and negative frequency modes compatible with deSitter invariance (known as α vacua) fails to define a Hadamard state. Perturbation theory in an α vacuum suffers from incurable UV divergences already at one loop order. One is thus led to search for Hadamard states on an FL background in the interval $(t_{\rm sing}, t_1]$ with implicitly defined bonus properties that lead to a qualitatively correct power spectrum at $t = t_*$. We propose massless SLE states as viable candidates.

5.5.1 Asymptotics of massless modes versus power spectrum

We return to the basic wave equation in conformal time (196) and specialize to the massless case and $d = 3$

$$\Big[\partial_\eta^2 + p^2 - \frac{\partial_\eta^2 a}{a}\Big]\chi_p(\eta) = 0\,, \quad \partial_\eta\chi_p\chi_p^* - (\partial_\eta\chi_p)^*\chi_p = -i\,. \tag{358}$$

The wave equation (358) bears a two-fold relation to lowest order cosmological perturbation theory, see e.g. [101], Chapter 10: (a) it coincides precisely with the wave equation satisfied by the tensor perturbations, with χ_p playing the role of either of the coefficient functions $h_+(\eta, p)$ or $h_\times(\eta, p)$ in the polarization decomposition $h_{ij}(\eta, x) = h_+(\eta, x)e_{ij}^+ + h_\times(\eta, x)e_{ij}^\times$, and $ds^2 = a(\eta)^2[-d\eta^2 + (\delta_{ij} + h_{ij})dx^i dx^j]$. (b) With the replacement of a by z, the Mukhanov-Sasaki variable, it coincides with wave equation satisfied by the scalar (curvature) perturbations, where χ_p is often denoted by $v_p(\eta) = z(\eta)\mathcal{R}_p(\eta)$.

The equation (358) can be solved for small p and large p as detailed in Sections 5.3.1 and 5.4.1, respectively. For small p one has a convergent power series expansion $\chi_p(\eta) = \sum_{n\geq 0}\chi_n(\eta)p^{2n}$, which corresponds to the massless case of (279). Since $\tau = \int^\eta ds\, a(s)^{-2}$ and $S_p(\eta) = \chi_p(\eta)/a(\eta)$, the leading order $S_0(\tau)$ from before (289) reads

$$\chi_0(\eta) = a(\eta)\Big[z_0 + w_0\int_{\eta_0}^\eta \frac{ds}{a(s)^2}\Big]\,, \quad w_0 z_0^* - w_0^* z_0 = -i\,. \tag{359}$$

The higher orders then are determined recursively by transcribing (281). Heuristically, the leading order can be expected to be a good approximation if $p \ll \partial_\eta a/a$, $p^2 \ll \partial_\eta(\partial_\eta a/a)$, so that $2p^2 \ll \partial_\eta^2 a/a$. In other words, the wavelength $1/p$ of the mode needs to be uniformly

much larger than the comoving Hubble distance $a/\partial_\eta a$. Under these conditions $\int^\eta ds\, a(s)^{-2} \propto 1/(pa(\eta)^2)$ (with a small constant of proportionality) is selfconsistent and shows that the second term in χ_0 will be decreasing in η, while the first term is increasing. With the replacement of $a(\eta)$ by $z(\eta)$ the same applies to the scalar perturbations. It must be stressed that the low momentum behavior (359) is not generic; there are relevant solutions with a different behavior, as highlighted by the SLE solution (362) below.

In order to transcribe the WKB ansatz (297) we note $\int_{\tau_i}^\tau d\tau' a(\tau')^2 = \eta - \eta_i$ and $\partial_\tau = a(\eta)^2\partial_\eta$, for $d = 3$. Specializing also (298) to $\omega_0(\eta) = 0$, $\omega_2(\eta) = a(\eta)^2$ the WKB solution for (358) reads

$$\begin{aligned} \chi_p(\eta) &\asymp_N \frac{e^{-ip(\eta-\eta_i)}}{\sqrt{2p}}\Big\{1 + \sum_{n\geq 1}(ip)^{-n}s_n(\eta)\Big\}\,, \\ \partial_\eta s_n &= \partial_\eta s_1 s_{n-1} + \frac{1}{2}\partial_\eta^2 s_{n-1}\,, \quad \partial_\eta s_1 = -\frac{1}{2}\frac{\partial_\eta^2 a}{a}\,. \end{aligned} \tag{360}$$

For the modulus square this gives $2p|\chi_p(\eta)|^2 \asymp_N 1 + p^{-2}\partial_\eta^2 a/(2a) + O(p^{-2})$, see (363). Heuristically, the WBK approximation is expected to be good in the regime opposite to (359), i.e. whenever the wave length $1/p$ of the mode is uniformly much smaller than the comoving Hubble distance $a/\partial_\eta a$, entailing $\partial_\eta^2 a/a \ll 2p^2$. Again, simply replacing $a(\eta)$ by $z(\eta)$ gives the corresponding result for the scalar perturbations.

The quantity of interest is the power spectrum at the time of seed formation η_*. Per tensor mode it is defined by

$$P_\chi(p) := \lim_{\eta\to\eta_*} \frac{p^3}{2\pi^2}\frac{|\chi_p(\eta)|^2}{a(\eta)^2}\,, \tag{361}$$

and similarly with z replacing a for the scalar perturbations. The time η_* is often identified with the Hubble crossing time η_p, defined by $(\partial_\eta a/a)(\eta_p) = p$. This lies in the cross-over region of the (η, p) plane not directly accessible via the small or large momentum expansions. A nearly scale invariant power spectrum is one where $P_\chi(p) \propto p^{-2\epsilon}$ for a small positive coefficient $\epsilon > 0$. As indicated, the power spectrum also depends on the choice of solution χ_p. The principles of QFT in curved spacetime require its large momentum behavior to be constrained by the Hadamard property. A necessary but by no means sufficient condition for a solution to be Hadamard it that it approaches a positive frequency wave for $p \to \infty$.

The low momentum behavior is somewhat constrained along the lines discussed at the end of Section 5.3. In the present context, an additional constraint arises from the requirement that $p^3|\chi_p(\eta)|^2/a(\eta)^2$ is approximately scale invariant in the cross-over region of the (η, p) plane.

The SLE have been shown to meet the first two criteria. Here we explore the satisfiability of the last requirement. We first note the low and high momentum behavior by appealing to the results from Sections 5.3.2 and 5.4.2. For the low momentum expansion the formulas (289), (290), (291) require as input the directly transcribed massless commutator function $\Delta_0(\eta, \eta') = \int_{\eta'}^{\eta} ds\, a(s)^{-2}$. It solves $(a(\eta)^2\partial_\eta)^2\Delta_0(\eta, \eta') = 0$, where the field redefinition is not yet taken into account. (The latter generates an effective mass term and the computation would have to proceed differently). This leads to

$$\frac{|\chi_p^{\mathrm{SLE}}(\eta)|^2}{a(\eta)^2} = \frac{\bar{a}}{2p} + O(p)\,, \qquad \bar{a} = \frac{\int d\eta\, a(\eta)^{-4} f^{\mathrm{conf}}(\eta)^2}{\int d\eta\, f^{\mathrm{conf}}(\eta)^2}\,, \tag{362}$$

and similarly for z replacing a. For large momentum the modulus square has the generic WKB asymptotics

$$\frac{|\chi_p^{\mathrm{SLE}}(\eta)|^2}{a(\eta)^2} \asymp \frac{1}{2pa(\eta)^2}\Big\{1 + \frac{1}{2p^2}\frac{\partial_\eta^2 a}{a} + O\Big(\frac{1}{p^4}\Big)\Big\}\,, \tag{363}$$

and similarly for z replacing a. As usual, the cross-over region needed for the power spectrum is not directly accessible via these expansions.

5.5.2 A model with pre-inflationary SLE

To proceed, we consider an analytically soluble model, adopted from [23], where the seed formation time η_* is p-independent and coincides with the end of a deSitter period. The deSitter period is preceded by one with kinetic energy domination. Computations of the power spectrum where a positive frequency solution in a pre-inflationary era is matched to a solution corresponding to accelerated expansion have been considered in [23, 86, 55, 25, 71].

Following [23], we use conformal time η and consider an instantaneous transition between

a kinetic dominated pre-inflationary period and de Sitter expansion. The scale factor reads

$$a(\eta) = \begin{cases} \sqrt{1+2H\eta}\,, & \eta \in (-\frac{1}{2H}, 0)\,, \\ \\ \frac{1}{1-H\eta}\,, & \eta \in [0, \frac{1}{H})\,, \end{cases} \tag{364}$$

with the transition occurring at $\eta_1 = 0$, and H denoting the (physical) Hubble parameter during inflation. The time of seed formation is $\eta_* = 1/H$ and the price to pay for the analytic solubility is the formal pole in the line element.

As seen in Section 5.2 the modulus square of an SLE solution is strictly independent of the choice of fiducial solution. We are thus free to choose a convenient one, $S_p(\eta) = \chi_p(\eta)/a(\eta)$, in the process of evaluating $|\chi_p^{\rm SLE}(\eta)/a(\eta)|^2$ for a given window function $f \in C_c^\infty(-1/(2H), 1/H)$. A useful choice adhering to the traditional Bunch-Davies solution during the deSitter period is

$$S_p(\eta) \;=\; \begin{cases} \alpha_p S_p^{\rm kin}(\eta) + \beta_p S_p^{\rm kin}(\eta)^*\,, & -\frac{1}{2H} < \eta \leq 0\,, \\ \\ S_p^{\rm BD}(\eta)\,, & 0 \leq \eta < \frac{1}{H}\,, \end{cases} \tag{365}$$

where

$$\begin{aligned} S_p^{\rm kin}(\eta) \;&:=\; \sqrt{\frac{\pi}{8H}}\, H_0^{(2)}\Big(p\eta + \frac{p}{2H}\Big)\,, \\ S_p^{\rm BD}(\eta) \;&:=\; \frac{e^{-ip(\eta-\frac{1}{H})}}{\sqrt{2p}}(1-H\eta)\Big(1 + \frac{iH}{p}\frac{1}{1-H\eta}\Big)\,, \end{aligned} \tag{366}$$

are solutions of (358) in their respective regimes. The matching coefficients $\alpha_p\,, \beta_p$ are determined by demanding continuity of S_p and $\partial_\eta S_p$ at the transition,

$$\begin{aligned} \alpha_p \;&=\; e^{ip/H}\sqrt{\frac{\pi p}{16H}}\Big[H_0^{(1)}\Big(\frac{p}{2H}\Big) - \Big(\frac{H}{p} - i\Big)H_1^{(1)}\Big(\frac{p}{2H}\Big)\Big]\,, \\ \beta_p \;&=\; e^{ip/H}\sqrt{\frac{\pi p}{16H}}\Big[-H_0^{(2)}\Big(\frac{p}{2H}\Big) + \Big(\frac{H}{p} - i\Big)H_1^{(2)}\Big(\frac{p}{2H}\Big)\Big]\,, \end{aligned} \tag{367}$$

with $|\alpha_p|^2 - |\beta_p|^2 = 1$ from the Wronskian condition.

This fiducial solution enters the SLE parameters c_1, c_2 and λ_p, μ_p from Section 5.2.1. The advantage of the choice (365) is that it leads to a relatively simple expression for the

power spectrum in terms of the (numerically computed) SLE parameters c_1 and c_2. The SLE solution will however *not* be of the Bunch-Davies type during the deSitter period,

$$\frac{\chi_p^{\rm SLE}(\eta)}{a(\eta)} = \lambda_p S^{\rm BD}(\eta) + \mu_p S^{\rm BD}(\eta)^* \,. \tag{368}$$

For $\eta_* = 1/H$ the SLE's power spectrum (361) is given by

$$P_{\chi^{\rm SLE}}(p) \;=\; \frac{H^2}{(2\pi)^2}|\lambda_p - \mu_p|^2 = \frac{H^2}{(2\pi)^2}\frac{c_1 + \Re c_2}{\sqrt{c_1^2 - |c_2|^2}} \,. \tag{369}$$

Here

$$\begin{aligned} c_1 \;&=\; \frac{1}{2}\int d\eta\, f(\eta)^2 a(\eta)^2 \Big\{ |\partial_\eta S_p(\eta)|^2 + p^2 |S_p(\eta)|^2 \Big\} \,, \\ c_2 \;&=\; \frac{1}{2}\int d\eta\, f(\eta)^2 a(\eta)^2 \Big\{ (\partial_\eta S_p(\eta))^2 + p^2 S_p(\eta)^2 \Big\} \,, \end{aligned} \tag{370}$$

are determined by (365). With some slight caveats it follows from the earlier results that the right hand side is indeed a Bogoliubov invariant: by (260) this holds for $\sqrt{c_1^2 - |c_2|^2}$ and since $\lim_{\eta_0 \to 1/H} S_p^{\rm BD}(\eta_0) = iH/\sqrt{2p^3}$ one can interpret the first line of (259) as $\lim_{\eta_0 \to 1/H} J_p(\eta_0) = (H^2/p^3)(c_1 + \Re c_2)$. Further, the relation (362) immediately suggests the low momentum asymptotics, while (363) in combination with $\lim_{\eta \to 1/H} a(\eta)^{-2} = 0$, $\lim_{\eta \to 1/H} a(\eta)^{-3}\partial_\eta^2 a = 2H^2$, suggests $\lim_{\eta \to 1/H} |\chi_p^{\rm SLE}(\eta)/a(\eta)|^2 = H^2/(2p^3) + O(p^{-5})$ for large p. The caveats are: that $\eta = 1/H$ lies at the boundary of the interval $[0, 1/H)$, that the line element (364) has a pole there, and that the window function may not have support in the deSitter phase only. We therefore present a more careful analysis of the small and large momentum behavior of $P_{\chi^{SLE}}(p)$, allowing for a generic window function with support in both the kinetic dominated and the deSitter period, thereby demonstrating that the above conclusions are indeed valid.

Proposition 5.5.1. Let $f \in C_c^\infty(-\frac{1}{2H}, \frac{1}{H})$ be a window function for (370). Then

$$(a) \qquad P_{\chi^{\rm SLE}}(p) = \frac{H^2}{(2\pi)^2} + O(p^{-2}) \;\text{ as }\; p \to \infty \,.$$

$$(b) \qquad P_{\chi^{\rm SLE}}(p) = p^2 \frac{\bar{a}}{(2\pi)^2} + O(p^4) \;\text{ as }\; p \to 0 \,.$$

Proof.

(a) The large p asymptotics are conveniently analyzed in terms of (369), where the λ_p, μ_p

coefficients refer to (365), (366), (367) as the fiducial solution for the SLE construction.

As the window function f is allowed to have support both in the kinetic dominated and de Sitter periods, it is convenient to split the integrations in (370)

$$c_1 = c_1^< + c_1^> \quad \text{and} \quad c_2 = c_2^< + c_2^> \,, \tag{371}$$

with the $<$ ($>$) denoting the contribution from the kinetic dominated (de Sitter) regime. This takes into account the distinct forms of our fiducial solution (365) in the respective regimes. We may readily read off

$$\begin{aligned} c_1^> &= \frac{p}{2}\int_0^{\frac{1}{H}} d\eta\, f(\eta)^2 a(\eta)^2 (1-H\eta)^2 + \frac{1}{2}\frac{H^2}{2p}\int_0^{\frac{1}{H}} d\eta\, f(\eta)^2 a(\eta)^2 \,, \\ c_2^> &= \frac{1}{2}\int_0^{\frac{1}{H}} d\eta\, f(\eta)^2 a(\eta)^2 e^{-2ip(\eta-\frac{1}{H})}\left[iH - iH^2\eta - \frac{H^2}{2p}\right]. \end{aligned} \tag{372}$$

For the analysis of the $c_1^<$, $c_2^<$ terms, it will prove helpful to define

$$\begin{aligned} \bar{c}_1 &:= \frac{1}{2}\int_{-\frac{1}{2H}}^0 d\eta\, f(\eta)^2 a(\eta)^2 \Big\{ |\partial_\eta S_p^{\rm kin}(\eta)|^2 + p^2 |S_p^{\rm kin}(\eta)|^2 \Big\} \,, \\ \bar{c}_2 &:= \frac{1}{2}\int_{-\frac{1}{2H}}^0 d\eta\, f(\eta)^2 a(\eta)^2 \Big\{ (\partial_\eta S_p^{\rm kin}(\eta))^2 + p^2 S_p^{\rm kin}(\eta)^2 \Big\} \,, \end{aligned} \tag{373}$$

in terms of which we may express

$$\begin{aligned} c_1^< &= (|\alpha_p|^2 + |\beta_p|^2)\bar{c}_1 + 2\Re\big[\alpha_p \beta_p^* \bar{c}_2\big] \,, \\ c_2^< &= \alpha_p^2 \bar{c}_2 + \beta_p^2 \bar{c}_2^{\,*} + 2\alpha_p\beta_p\bar{c}_1 \,. \end{aligned} \tag{374}$$

The $e^{-2ip(\eta-\frac{1}{H})}$ term in the integrand of $c_2^>$ entails that $c_2^> \sim O(p^{-n})$ for any $n \in \mathbb{N}$ as $p \to \infty$. Hence, $c_2^>$ is negligible compared to $c_1^>$, for large enough p. Next, in order to understand the asymptotic behavior of (373), (374), it is sufficient to consider the leading asymptotic behavior of $S_p^{\rm kin}(\eta)$ as $p \to \infty$,

$$S_p^{\rm kin}(\eta) \sim \frac{1}{\sqrt{4Hp}}\left(\eta + \frac{1}{2H}\right)^{-\frac{1}{2}} e^{-ip(\eta+\frac{1}{2H})+i\pi/4}\big(1+O(p^{-1})\big) \,, \tag{375}$$

leading to

$$\begin{aligned}\bar{c}_1 &\sim \frac{p}{2}\int_{-\frac{1}{2H}}^{0} d\eta\, f(\eta)^2\,, \qquad (376)\\ \bar{c}_2 &\sim \frac{1}{2}\int_{-\frac{1}{2H}}^{0} d\eta\, f(\eta)^2 a(\eta)^2 e^{-2ip(\eta+\frac{1}{2H})}\left[\frac{H}{(1+2H\eta)^2}-\frac{iH}{2p(1+2H\eta)^3}\right]\left(1+O(p^{-1})\right).\end{aligned}$$

As before, the presence of the $e^{-2ip(\eta+\frac{1}{2H})}$ entails that $\bar{c}_2 \ll \bar{c}_1$ as $p\to\infty$.

Using (374) to express $|c_2|^2/c_1^2$ in terms of $c_1^>$, $c_2^>$, $\bar{c}_1$, $\bar{c}_2$, we may disregard relative contributions of $c_2^>, \bar{c}_2$ to $|c_2|^2/c_1^2$, and find

$$\begin{aligned}|c_2|^2 &= 4|\beta_p|^2(1+|\beta_p|^2)\bar{c}_1^2\,,\\ c_1^2 &= (\bar{c}_1+c_1^>)^2+4|\beta_p|^2\big[(1+|\beta_p|^2)\bar{c}_1^2+|\beta_p|^2\bar{c}_1 c_1^>\big]\,, \qquad (377)\end{aligned}$$

where we have used the fact that $|\alpha_p|^2-|\beta_p|^2=1$ to write α_p in terms of β_p. Examining (372) and (376), it is clear that $\bar{c}_1$ and $c_1^>$ have the same leading large p behavior, and from (367) it follows that $|\beta_p|^2 \sim \frac{9H^4}{16p^4}+O(p^{-6})$. Thus we use (377) to estimate

$$\frac{|c_2|^2}{c_1^2} \sim O(p^{-4})\,. \qquad (378)$$

Since

$$\mu_p = \frac{1}{\sqrt{2}}\sqrt{\frac{1}{1-\frac{|c_2|^2}{c_1^2}}-1}\,, \quad |\lambda_p| = \sqrt{1+\mu_p^2}\,, \qquad (379)$$

this establishes part (a) of Proposition 5.5.1.

(b) The main obstruction to using (362) to infer the result is that the limit $\eta\to 1/H$ of the small p SLE expansion is not a-priori well-defined. We remove this obstruction by a small modification of Proposition 5.3.1.

In both the kinetic dominated and deSitter regimes, the mode equation reads $S_p''(\eta)+2\frac{a'}{a}S_p'(\eta)+p^2S_p(\eta)=0$. Consistent with (359) we choose the following solution for the $p=0$

equation

$$S_0(\eta) = \begin{cases} \frac{1}{\sqrt{2}}\Big[\frac{\ln(1+2H\eta)}{2H} - \frac{1}{3H} + i\Big]\,, & \text{kinetic domination}\,, \\ \frac{1}{\sqrt{2}}\Big[-\frac{1}{3H}(1-H\eta)^3 + i\Big]\,, & \text{deSitter}\,. \end{cases} \tag{380}$$

Both cases satisfy $[\partial_\eta S_0\, S_0^* - S_0\, \partial_\eta S_0^*](\eta) = -ia(\eta)^{-2}$, as well as

$$\lim_{\eta\to 1/H} S_0(\eta) = \frac{i}{\sqrt{2}} \quad \text{and} \quad \lim_{\eta\to 1/H} \partial_\eta S_0(\eta) = 0\,. \tag{381}$$

This shows that S_0 extends uniquely to a continuous function on $(-1/(2H),\, 1/H]$.

Choosing some $0 < \eta_i < 1/H$ such that $\operatorname{supp} f \subset [\eta_i,\, 1/H]$, it clear that a solution of the integral equation

$$\begin{aligned} S(\eta) &= S_0(\eta) - p^2 \int_{\eta_i}^{1/H} K(\eta,\eta') S(\eta') d\eta'\,, \\ K(\eta,\eta') &= i\theta(\eta-\eta') S_0(\eta) S_0(\eta')^* + \theta(\eta'-\eta) S_0(\eta)^* S_0(\eta')\,, \end{aligned} \tag{382}$$

is a solution of the mode equation on $(\eta_i, 1/H)$. Since S_0 extends to a C^1 function on the closed interval $[\eta_i,\, 1/H]$, the proof of Proposition 5.3.1 carries over on the Banach space $\big(C([\eta_i, 1/H], \mathbb{C}^2),\, \|\cdot\|_{\sup}\big)$.

Hence we have a convergent series $S_p(\eta) = \sum_{n=0}^\infty p^{2n} S_n(\eta)$, which we take as the fiducial solution for the SLE in the small p regime. This then has a well-defined limit as $\eta \to 1/H$, namely

$$\begin{aligned} \lim_{\eta\to 1/H} T_p^{\text{SLE}}(\eta) &= \lambda_p \lim_{\eta\to 1/H} S_p(\eta) + \mu_p \lim_{\eta\to 1/H} S_p(\eta)^* \\ &= \lambda_p S_p(1/H) + \mu_p S_p(1/H)^*\,. \end{aligned} \tag{383}$$

Both $p^{\frac{1}{2}}\lambda_p$ and $p^{\frac{1}{2}}\mu_p$ admit convergent power series expansions as in (295), leading to

$$|T_p^{\text{SLE}}(1/H)| = \frac{\bar{a}}{2p} + O(p)\,, \tag{384}$$

which proves part (b). □

The proposition provides an analytical description of the power spectrum's small and large momentum behavior. For intermediate momenta we evaluate $\chi_p^{\text{SLE}}(\eta)$ numerically. For

the numerical implementation a choice of window function in $C_c^\infty(-\frac{1}{2H}, \frac{1}{H})$ enters. A useful one-parametric family arises as follows. From the standard smoothened step function

$$h(y) := \begin{cases} 0 & y \leq 0\,, \\ \frac{e^{-1/y}}{e^{-1/y}+e^{-1/(1-y)}} & 0 < y < 1\,, \\ 1 & y \geq 1\,, \end{cases} \tag{385}$$

we define the bump function of width $1 + w$ centered at the origin,

$$\texttt{bump}(y, w) := 1 - h\left(\frac{y^2 - w^2}{(w+1)^2 - w^2}\right), \tag{386}$$

where w is the ratio of "plateau" of the bump to the "walls" of the bump. Finally we define

$$F(\eta, \eta_1, \eta_2; w) := \texttt{bump}\left(\frac{\eta - (\frac{\eta_1+\eta_2}{2})}{\frac{\eta_1+\eta_2}{2(w+1)}}, w\right), \tag{387}$$

a positive smoothened "top hat" function centered at $\frac{\eta_1+\eta_2}{2}$. Here $\eta_1 < \eta_2$ are the "ends" of the hat, specifying the cosmological period over which $F = (f^{\text{cosm}})^2$ has support. The results of the power spectrum for various values of η_1, η_2 and $w = 0.5$ are shown in the following figure

5.6 Generalized States of Low Energy

The SLE discussed in the previous sections are exact Hadamard states, and have the physically appealing "average energy minimization" property. Moreover, the SLE construction (223)-(225) has the feature of "elevating" any fiducial solution S of (193) to a unique[3] Hadamard state. As far as the Hadamard property is concerned, however, this minimization is far from necessary on a mathematical level. We shall demonstrate this by generalizing the SLE construction to a simple one-parameter family of homogeneous quasi-free states for the Klein-Gordon field of mass $m > 0$ on Friedmann-Lemaître spacetimes that are (1) unique, and (2) exact Hadamard states, depending on a freely specifiable parameter M.

[3]Unique up to the choice of the window function f.

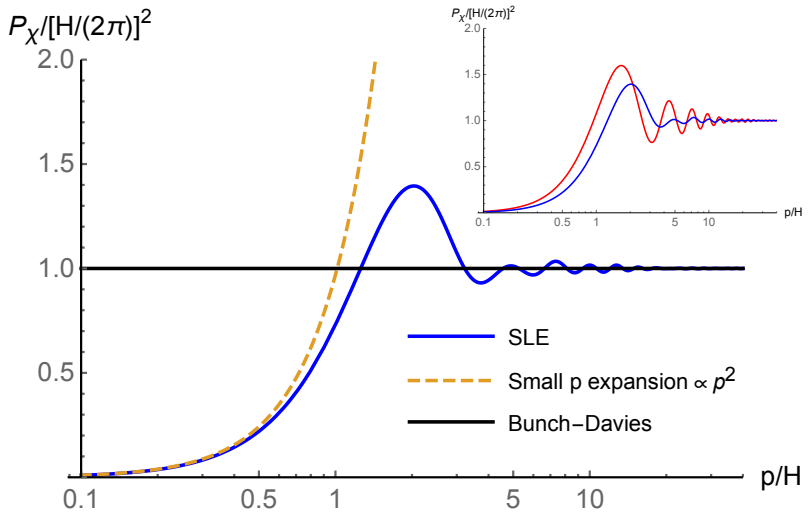


Figure 5: Power spectrum for a primordial SLE and window function (387) with support in $[-0.3, 0.5]/H$. The insert shows in red the comparison with a situation where the window function has support in the pre-inflationary period $[-0.3, 0]/H$ only.

We begin with the (spatially Fourier transformed) Klein-Gordon equation (193) with mass M instead of m,

$$\begin{aligned} &\big[\partial_\tau^2 + \omega_{p,\mathrm{M}}(\tau)^2\big] S_{p,\mathrm{M}}(\tau) = 0\,, \quad \omega_{p,\mathrm{M}}(\tau)^2 := a(\tau)^{2d}\mathrm{M}^2 + p^2 a(\tau)^{2d-2}\,, \\ &\partial_\tau S_{p,\mathrm{M}}\, S^*_{p,\mathrm{M}} - \partial_\tau S^*_{p,\mathrm{M}}\, S_{p,\mathrm{M}} = -i\,. \end{aligned} \tag{388}$$

A solution will parametrically depend on p and M, which we indicate by a subscript, $S_{p,\mathrm{M}}$. This mass $\mathrm{M} \geq 0$ need not *a priori* have any relation to the particle mass m in (193), except that we obtain a vacuum state of our original theory through the specialization $S_{p,\mathrm{M}=m}$. To distinguish these, we shall refer to solutions of the original wave equation (193) as "m-modes", and solutions of (388) as "M-modes".

For a fiducial M-mode $S_{p,\mathrm{M}}$, the Bogoliubov coefficients $(\lambda[S], \mu[S])_{p,\mathrm{M}}$ yielding the M-SLE $T^{\mathrm{SLE}}_{p,\mathrm{M}}$ that minimizes the M-mode smeared energy,

$$\mathcal{E}_{p,\mathrm{M}}[T^{\mathrm{SLE}}] := \int d\tau\, f(\tau)^2 \Big\{ |\partial_t T^{\mathrm{SLE}}_{p,\mathrm{M}}(\tau)|^2 + \omega_{p,\mathrm{M}}(\tau)^2 |T^{\mathrm{SLE}}_{p,\mathrm{M}}(\tau)|^2 \Big\}\,, \tag{389}$$

are clearly those in (225), with the particle mass m^2 replaced by the deformed mass scale M^2. Given these Bogoliubov coefficients, we define the Generalized State of Low Energy (GLSE) solution of (193) with fiducial solution S,

$$T_{p,m,\mathrm{M}}[S](\tau) := \lambda_{p,\mathrm{M}}[S]S_{p,\mathrm{M}=m}(\tau) + \mu_{p,\mathrm{M}}[S]S_{p,\mathrm{M}=m}(\tau)^*\,, \tag{390}$$

which depends on both m and M. For $\mathrm{M} = m$ this is the standard SLE and is hence independent of the choice of fiducial solution by Theorem 5.2.1. However, the above proof only applies to the SLE proper, and hence the GLSE off-hand might depend on the choice of fiducial solution S used to realize it. We address this in the following theorem:

Theorem 5.6.1 (Uniqueness of GSLE)**.**

The GSLE two-point function based on a fiducial solution S

$$W[S](\tau, x; \tau', x') := \int \frac{d^d p}{(2\pi)^d} e^{ip(x-x')} T_{p,m,\mathrm{M}}[S](\tau) T_{p,m,\mathrm{M}}[S](\tau')^*\,, \tag{391}$$

is a Bogoliubov invariant, i.e. $W[aS + bS^*] = W[S]$ with $a, b \in \mathbb{C}$, $|a|^2 - |b|^2 = 1$. Hence the GSLE defines a homogeneous pure quasi-free, independent of the choice of fiducial solution used to realize it.

Proof.

In the proof presented in Section 5.2.2 (as well as in [80]) the claimed Bogoliubov invariance follows from the minimization property of the SLE. Here we present a simple algebraic argument that is more general, resting on the Bogoliubov transformation properties of the functionals $\mathcal{E}_{p,\mathrm{M}}$, $\mathcal{D}_{p,\mathrm{M}}$.

Let $S_{p,\mathrm{M}}$ and $\tilde{S}_{p,\mathrm{M}}$ be two fiducial solutions of (388), related by a Bogoliubov transformation

$$S_{p,\mathrm{M}}(\tau) \;=\; a\tilde{S}_{p,\mathrm{M}}(\tau) + b\tilde{S}_{p,\mathrm{M}}(\tau)^*\,, \quad a, b \in \mathbb{C}, \quad |a|^2 - |b|^2 = 1\,, \tag{392}$$

and

$$\begin{aligned}
\mathcal{E}_{p,\mathrm{M}}[S] \;&=\; \int d\tau\, f(\tau)^2 \Big\{ |\partial_\tau S_{p,\mathrm{M}}(\tau)|^2 + \omega_{p,\mathrm{M}}(\tau)^2 |S_{p,\mu}(\tau)|^2 \Big\}\,, \\
\mathcal{D}_{p,\mathrm{M}}[S] \;&=\; \int d\tau\, f(\tau)^2 \Big\{ (\partial_t S_{p,\mathrm{M}}(\tau))^2 + \omega_{p,\mathrm{M}}(\tau)^2 S_{p,\mathrm{M}}(\tau)^2 \Big\}\,.
\end{aligned} \tag{393}$$

Since we shall (until further notice) be concerned exclusively with the M-modes, we omit the p, M subscripts. These will be reinstated once again when the distinction from the m-modes is necessary.

Observe that the functionals $\mathcal{E}$, $\mathcal{D}$ can be understood as the diagonal of two bi-functionals,

$$\mathcal{E}[S] \;=\; C_1(S,S)\,, \quad \mathcal{D}[S] = C_2(S,S)\,, \tag{394}$$

with C_1 sesquilinear and C_2 bilinear, which are related by $C_1(S^*,S) = C_2(S,S)$ and $C_2(S^*,S) = C_1(S,S)$. Inserting the Bogoliubov transformation (392), application of bi/sesqui-linearity yields

$$\begin{aligned} C_1(a\tilde{S}+b\tilde{S}^*, a\tilde{S}+b\tilde{S}^*) \;&=\; |a|^2 C_1(\tilde{S},\tilde{S}) + a^*b C_1(\tilde{S},\tilde{S}^*) + ab^* C_1(\tilde{S}^*,\tilde{S}) + |b|^2 C_1(\tilde{S}^*,\tilde{S}^*) \\ &=\; (|a|^2+|b|^2) C_1(\tilde{S},\tilde{S}) + a^*b C_2(\tilde{S},\tilde{S})^* + ab^* C_2(\tilde{S},\tilde{S}) \\ &=\; (|a|^2+|b|^2)\mathcal{E}[\tilde{S}] + ab^*\mathcal{D}[\tilde{S}] + a^*b\mathcal{D}[\tilde{S}]^*\,, \end{aligned} \tag{395}$$

$$\begin{aligned} C_2(a\tilde{S}+b\tilde{S}^*, a\tilde{S}+b\tilde{S}^*) \;&=\; a^2 C_2(\tilde{S},\tilde{S}) + abC_2(\tilde{S},\tilde{S}^*) + abC_2(\tilde{S}^*,\tilde{S}) + b^2 C_2(\tilde{S}^*,\tilde{S}^*) \\ &=\; a^2 C_2(\tilde{S},\tilde{S}) + b^2 C_2(\tilde{S},\tilde{S})^* + 2ab C_1(\tilde{S},\tilde{S}) \\ &=\; a^2\mathcal{D}[\tilde{S}] + b^2\mathcal{D}[\tilde{S}]^* + 2ab\mathcal{E}[\tilde{S}]\,. \end{aligned} \tag{396}$$

In summary, under a Bogoliubov transformation, the functionals $\mathcal{E}$ and $\mathcal{D}$ therefore transform as

$$\begin{aligned} \mathcal{E}[a\tilde{S}+b\tilde{S}^*] \;&=\; (|a|^2+|b|^2)\mathcal{E}[\tilde{S}] + ab^*\mathcal{D}[\tilde{S}] + a^*b\mathcal{D}[\tilde{S}]^*\,, \\ \mathcal{D}[a\tilde{S}+b\tilde{S}^*] \;&=\; a^2\mathcal{D}[\tilde{S}] + b^2\mathcal{D}[\tilde{S}]^* + 2ab\mathcal{E}[\tilde{S}]\,. \end{aligned} \tag{397}$$

and hence

$$\mathcal{E}[a\tilde{S}+b\tilde{S}^*]^2 - |\mathcal{D}[a\tilde{S}+b\tilde{S}^*]|^2 \;=\; (|a|^2-|b|^2)(\mathcal{E}[\tilde{S}]^2 - |\mathcal{D}[\tilde{S}]|^2) = \mathcal{E}[\tilde{S}]^2 - |\mathcal{D}[\tilde{S}]|^2\,, \tag{398}$$

i.e. $\mathcal{E}[S]^2 - |\mathcal{D}[S]|^2$ is Bogoliubov invariant.

Now we consider the GSLE $T_{p,m,\mathrm{M}}$ determined by mode function $S_{p,\mathrm{M}}$,

$$T_{p,m,\mathrm{M}}[S](\tau) \;\;=\;\; \lambda_{p,\mathrm{M}}[S] S_{p,\mathrm{M}=m}(\tau) + \mu_{p,\mathrm{M}}[S] S_{p,\mathrm{M}=m}(\tau)^*\,,$$

$$\begin{aligned}\left|T_{p,m,\mathrm{M}}[S](\tau)\right|^2 &= (|\lambda_{p,\mathrm{M}}[S]|^2+\mu_{p,\mathrm{M}}[S]^2)|S_{p,\mathrm{M}=m}(\tau)|^2 \\ &+ \lambda_{p,\mathrm{M}}[S]\mu_{p,\mathrm{M}}[S]S_{p,\mathrm{M}=m}(\tau)^2+\lambda_{p,\mathrm{M}}[S]^*\mu_{p,\mathrm{M}}[S]S_{p,\mathrm{M}=m}(\tau)^{*\,2} \\ &= \frac{1}{2\sqrt{\mathcal{E}_{p,\mathrm{M}}[S]^2-|\mathcal{D}_{p,\mathrm{M}}[S]|^2}}\big\{2\mathcal{E}_{p,\mathrm{M}}[S]\left|S_{p,\mathrm{M}=m}(\tau)\right|^2 \\ &- \mathcal{D}_{p,\mathrm{M}}[S]^*S_{p,\mathrm{M}=m}(\tau)^2-\mathcal{D}_{p,\mathrm{M}}[S]S_{p,\mathrm{M}=m}(\tau)^{*\,2}\big\}. \end{aligned} \tag{399}$$

Inserting the transformation (392), together with (397), (398) yields

$$\begin{aligned}\left|T_{p,m,\mathrm{M}}[a\tilde{S}+b\tilde{S}^*](\tau)\right|^2 &= \frac{|a|^2-|b|^2}{2\sqrt{\mathcal{E}_{p,\mathrm{M}}[\tilde{S}]^2-|\mathcal{D}_{p,\mathrm{M}}[\tilde{S}]|^2}}\Big\{2\mathcal{E}_{p,\mathrm{M}}[\tilde{S}]\left|\tilde{S}_{p,\mathrm{M}=m}(\tau)\right|^2 \\ &- \mathcal{D}_{p,\mathrm{M}}[\tilde{S}]^*\tilde{S}_{p,\mathrm{M}=m}(\tau)^2-\mathcal{D}_{p,\mathrm{M}}[\tilde{S}]\tilde{S}_{p,\mathrm{M}=m}(\tau)^{*\,2}\Big\} \\ &= (|a|^2-|b|^2)\left|T_{p,m,\mathrm{M}}[\tilde{S}](\tau)\right|^2 \\ &= \left|T_{p,m,\mathrm{M}}[\tilde{S}](\tau)\right|^2, \end{aligned} \tag{400}$$

establishing Bogoliubov invariance.

□

5.6.1 GSLE are Hadamard states

Having established that the GSLE are well-defined vacua, we now turn to the question of their physical viability, established by the following theorem:

Theorem 5.6.2.

Let ω_2 be the homogeneous pure quasifree state associated to the GSLE mode functions $T_{p,m,\mathrm{M}}$ in (390). Then ω_2 has the Hadamard property.

We shall refer to these vacuum states as Generalized States of Low Energy and write $\omega_2=\omega_2^{\mathrm{GSLE}}$.

Radzikowski [87] gave a geometrical reformulation of the original definition of a Hadamard state by Kay and Wald [60] in terms of the wavefront set of its two-point distribution.

Definition 5.6.1.

Consider the Klein-Gordon equation on a globally hyperbolic manifold M, with algebra

of observables $\mathcal{A}(M)$. A quasifree state ω on the $\mathcal{A}(M)$ is said to be a *Hadamard state* if the wavefront set of its two-point distribution ω_2 satisfies $\mathrm{WF}(\omega_2) = C^+$, where C^+ is a subset of $T^*(M \times M)$, the cotangent bundle over $M \times M$, defined as

$$C^+ := \left\{(y_1, \xi_1; y_2, -\xi_2) \in T^*(M \times M) \setminus \{0\} \middle| (y_1, \xi_1) \sim (y_2, \xi_2),\, \xi_1 \in \overline{V}_+ \right\}, \tag{401}$$

Here the relation $(y_1, \xi_1) \sim (y_2, \xi_2)$ means that there exists a null-geodesic in M connecting y_1 and y_2, ξ_1 is the covector to this geodesic at y_1, and $\xi_2 \in T^*_{y_2}M$ is the parallel transport of ξ_1 along the geodesic. Finally, $\overline{V}_+$ is the closed forward lightcone of $T^*_{y_1}M$.

The wavefront set of a distribution captures not only the location of the distribution's singularities, but also the direction(s) in which they are propagated. While this definition of the Hadamard property is seemingly more abstract than the original formulation in terms of the Hadamard parametrix, modern formulations of QFT on curved spacetimes use Definition 5.6.1 due to its suitability for mathematical analysis.

Our proof that the GSLE are Hadamard states, i.e. $\mathrm{WF}(\omega_2^{\mathrm{GSLE}}) = C^+$, proceeds along by-now standard lines [80, 96, 17]. In order to show that the wavefront set of the GSLE coincides with that of a generic Hadamard state, we use adiabatic vacuum states as a "conduit" by appealing to a result of Junker-Schrohe [56] that establishes a connection between the Sobolev wavefront sets of adiabatic vacuum states and a generic Hadamard state. Specifically we shall show that the Sobolev wavefront sets of the GSLE coincides with that of the adiabatic vacua of sufficiently high orders, and hence (by the aforementioned result of Junker-Schrohe) coincides with the Sobolev wavefront set of a generic Hadamard state.

5.6.1.1 A brief wavefront set glossary

We present a brief overview of the aspects of wavefront sets required for the proof of the Hadamard property for the GSLE, referring to [61, 95] for a more detailed treatment.

To introduce the notion of the wavefront set consider a distribution on $\mathbb{R}^n$, $u \in \mathcal{D}'(\mathbb{R}^n)$[4]. This distribution may be "localized" about some $y_0 \in \mathbb{R}^n$ by multiplying with some $h \in C_c^\infty(\mathbb{R}^n)$ with $h(y_0) \neq 0$, yielding a distribution hu of compact support. Now suppose

[4]Here $\mathcal{D}'(\mathbb{R}^n)$, the space of distributions, is the topological dual of $\mathcal{D}(\mathbb{R}^n) \equiv C_c^\infty(\mathbb{R}^n)$.

that this distribution were smooth, i.e. $hu \in C_c^\infty(\mathbb{R}^n)$. Then it is a standard property of the Fourier transform that $(hu)^\wedge$ and all its derivatives are smooth and rapidly decreasing. Conversely, the failure of u to be smooth in a neighborhood of y_0 translates to a failure of the smoothness and rapid descent properties of $(hu)^\wedge$ in certain directions in Fourier space. This singularity structure of u is quantified in its C^∞-wavefront set $\mathrm{WF}(u)$, which identifies both the *locations* of the singularity, as well as the *directions* in which they propagate.

We now present the definition of the C^∞-wavefront set on $\mathbb{R}^n$. Due its local character, the generalization to smooth manifolds follows straightforwardly through the use of coordinate charts.

Definition 5.6.2 (The C^∞-wavefront set of a distribution)**.**

Let $u \in \mathcal{D}'(U)$ with $U \subseteq \mathbb{R}^n$ open. A point $(y_0, \xi_0) \in T^*\mathbb{R}^n$ is called a *regular directed point of* u if there exists $h \in C_c^\infty(\mathbb{R}^n)$ and an open conic neighborhood Γ_{ξ_0} of ξ_0 in $T_y^*\mathbb{R}^n \cong \mathbb{R}^n$, such that for every $n \in \mathbb{N}$ there is $C_n > 0$ and

$$\sup_{\xi \in \Gamma_{\xi_0}} \left|(hu)^\wedge(\xi)\right| \leq C_n(1 + |\xi|)^{-n} \,. \tag{402}$$

The C^∞-wavefront set $\mathrm{WF}(u)$ is then defined as the complement of the set of regular directed points in $T^*\mathbb{R}^n \setminus \{0\}$.

An important property of wavefront sets is their behavior when considering the sum of distributions, namely

$$\mathrm{WF}(u + v) \subseteq \mathrm{WF}(u) \cup \mathrm{WF}(v) \,. \tag{403}$$

Although the C^∞-wavefront set is sufficient to characterize the Hadamard property, it is advantageous to consider also the Sobolev wavefront sets WF^s. These contain information about the *degree* of a distribution's singularities, in addition to their location and direction. Sobolev wavefront sets were used in [56] to rigorously define adiabatic vacuum states, as well as characterize their relation to Hadamard states.

Sobolev spaces generalize the notion of a derivative to L^p spaces through the weak-derivative. For L^2 spaces an equivalent characterization may be given through the Fourier transform. The essential notion is that of a *local Sobolev space* H^s_{loc}.

Definition 5.6.3 (Local Sobolev spaces)**.**

First we consider $\mathbb{R}^n$, where for $s \in \mathbb{R}$

$$H^s_{\mathrm{loc}}(\mathbb{R}^n) := \Big\{ u \in \mathcal{D}'(\mathbb{R}^n) \,\Big|\, \forall\, h \in C^\infty_c(\mathbb{R}^n) : \int d^n\xi\, (1+|\xi|^2)^s |(hu)^\wedge(\xi)|^2 < \infty \Big\}\,, \tag{404}$$

where $\mathcal{D}'(\mathbb{R}^N)$ is the topological dual of $C^\infty_c(\mathbb{R}^N)$.

Next, let M be an arbitrary smooth manifold. Then we say that $u \in \mathcal{D}'(M)$ is in $H^s_{\mathrm{loc}}(M)$ for $s \in \mathbb{R}$ if for any chart (U, Φ) and any $h \in C^\infty_c(U)$

$$\int d^n\xi\, (1+|\xi|^2)^s |(\Phi^*(hu))^\wedge(\xi)| < \infty\,, \tag{405}$$

with Φ^* denoting the pull-back. Recall that $\mathcal{D}'(M)$ is the topological dual of $C^\infty_c(M)$.

The Sobolev wavefront set is defined as usual through a complement:

Definition 5.6.4 (Sobolev wavefront set)**.**

Let $u \in \mathcal{D}'(\mathbb{R}^n)$, $y_0 \in \mathbb{R}^n$, $\xi \in \mathbb{R}^n \setminus \big\{0\big\}$ and $s \in \mathbb{R}$. Then $(y_0, \xi_0) \notin \mathrm{WF}^s(u)$ if there exists $h \in C^\infty_c(\mathbb{R}^n)$ with $h(y_0) \neq 0$ and an open conic neighborhood Γ of $\xi_0 \in \mathbb{R}^N \setminus \big\{0\big\}$ such that

$$\int_\Gamma d^N\xi\, (1+|\xi|^2)^s |(\varphi u)^\wedge(\xi)|^2 < \infty\,. \tag{406}$$

The generalization to smooth manifolds through the use of charts is immediate.

We end this glossary with a few remarks.

Remarks:

(1) It is clear that $\mathrm{WF}^s(u) = \emptyset$ is equivalent to $u \in H^s_{\mathrm{loc}}(M)$. It also follows from the definition (404), (405) of local Sobolev spaces and standard properties of the Fourier transform that all functions of sufficiently high differentiability are contained therein, specifically

$$\forall\, s < j - \tfrac{1}{2}\dim(M) :\, C^j(M) \subseteq H^s_{\mathrm{loc}}(M)\,, \tag{407}$$

with the $\frac{1}{2}\dim(M)$ arising from the measure in (405).

(2) The analog of (403) for the Sobolev wavefront sets is

$$\forall\, s \in \mathbb{R} :\, \mathrm{WF}^s(u+v) \subseteq \mathrm{WF}^s(u) \cup \mathrm{WF}^s(v)\,. \tag{408}$$

(3) The C^∞-wavefront set is related to the Sobolev wavefront sets by

$$\mathrm{WF}(u) = \overline{\bigcup_{s\in\mathbb{R}} \mathrm{WF}^s(u)}\,. \tag{409}$$

5.6.1.2 Proof of the Hadamard property of the GSLE

We begin with the definition of the adiabatic iteration and adiabatic vacua, adapted from [68]. Inserting the WKB ansatz

$$S_{p,\mathrm{M}}(\tau) = \frac{1}{\sqrt{2\Omega_{p,\mathrm{M}}(\tau)}} \exp\Big\{ -i \int^\tau d\tau'\, \Omega_{p,\mathrm{M}}(\tau') \Big\} \tag{410}$$

into (388) yields the following relation for the frequency

$$\Omega_{p,\mathrm{M}}(\tau)^2 \;=\; \omega_{p,\mathrm{M}}(\tau)^2 + \Big[\frac{3(\partial_\tau \Omega_{p,\mathrm{M}})^2}{4\Omega_{p,\mathrm{M}}^2} - \frac{\partial_\tau^2 \Omega_{p,\mathrm{M}}}{2\Omega_{p,\mathrm{M}}} \Big](\tau)\,. \tag{411}$$

Solving this iteratively yields the recursion

$$(\Omega^{(0)}_{p,\mathrm{M}})^2 := \omega_{p,\mathrm{M}}(\tau)^2\,, \quad (\Omega^{(n+1)}_{p,\mathrm{M}})^2 \;=\; \omega_{p,\mathrm{M}}(\tau)^2 + \Big[\frac{3(\partial_\tau \Omega^{(n)}_{p,\mathrm{M}})^2}{4(\Omega^{(n)}_{p,\mathrm{M}})^2} - \frac{\partial_\tau^2 \Omega^{(n)}_{p,\mathrm{M}}}{2\Omega^{(n)}_{p,\mathrm{M}}} \Big](\tau)\,, \tag{412}$$

and thereby the adiabatic iterate of order $n \in \mathbb{N}_0$

$$W^{(n)}_{p,\mathrm{M}}(t) = \frac{1}{\sqrt{2\Omega^{(n)}_{p,\mathrm{M}}(t)}} \exp\Big\{ -i \int^\tau d\tau' \Omega^{(n)}_{p,\mathrm{M}}(\tau') \Big\}\,. \tag{413}$$

We remark that as long as $\mathrm{M}^2 > 0$ the iteration procedure (412) yields well-defined $\Omega^{(n)}_{p,\mathrm{M}}$ for all $n \in \mathbb{N}_0$ and momenta p (which may, however, be complex for small p). The adiabatic iterates $W^{(n)}_{p,\mathrm{M}}$ are therefore also well-defined for all p (though not a genuine solution of (388)). An exact solution $S^{(n)}_{p,\mathrm{M}}$ of (388), *the adiabatic mode of order* $n \in \mathbb{N}_0$, may be defined by using the iterates (413) as initial data on a Cauchy surface at time coordinate τ_0,

$$S^{(n)}_{p,\mathrm{M}}(\tau_0) \stackrel{!}{=} W^{(n)}_{p,\mathrm{M}}(\tau_0)\,, \quad \partial_\tau S^{(n)}_{p,\mathrm{M}}(\tau_0) \stackrel{!}{=} \partial_\tau W^{(n)}_{p,\mathrm{M}}(\tau_0)\,. \tag{414}$$

For $\mathrm{M}^2 > 0$ the adiabatic modes $S^{(n)}_{p,\mathrm{M}}$ are well-defined for all momenta. Moreover, the adiabatic vacua $S^{(n)}_{p,\mathrm{M}}$ may be expressed in terms of the adiabatic iterates $W^{(n)}_{p,\mathrm{M}}$,

$$S^{(n)}_{p,\mathrm{M}}(\tau) \;=\; \alpha^{(n)}_{p,\mathrm{M}}(\tau) W^{(n)}_{p,\mathrm{M}}(\tau) + \beta^{(n)}_{p,\mathrm{M}}(\tau) W^{(n)}_{p,\mathrm{M}}(\tau)^*\,. \tag{415}$$

An argument along the lines of the proof of Lemma 5.4.1 yields the estimates

$$\begin{aligned}\alpha^{(n)}_{p,\mathrm{M}}(\tau) &= 1 + O(p^{-2n-1})\,, \quad \partial_\tau \alpha^{(n)}_{p,\mathrm{M}}(\tau) = O(p^{-2n-1})\,,\\ \beta^{(n)}_{p,\mathrm{M}}(\tau) &= O(p^{-2n-1})\,, \quad \partial_\tau \beta^{(n)}_{p,\mathrm{M}}(\tau) = O(p^{-2n-1})\,.\end{aligned} \tag{416}$$

In turn these imply the following estimates on the large momentum asymptotics of the adiabatic modes,

$$S^{(n)}_{p,\mathrm{M}}(\tau) = O(p^{-1/2})\,, \quad \partial_\tau S^{(n)}_{p,\mathrm{M}}(\tau) = O(p^{1/2})\,, \quad \forall\, j \geq 2 :\, \partial^j_\tau S^{(n)}_{p,\mathrm{M}}(\tau) = O(p^{j-1/2})\,, \tag{417}$$

with the final estimate following from the first two by repeated differentiation of (388).

Having introduced the adiabatic vacua of order n, we may use these as fiducial solutions for the construction of the GSLE, assured by Theorem 5.6.1 that the resulting state is independent of the choice of adiabatic order. Given an adiabatic mode of order $n \in \mathbb{N}_0$, the proof of Lemma 4.5 in [80] shows that $\lambda_{p,\mathrm{M}}[S^{(n)}]$, $\mu_{p,\mathrm{M}}[S^{(n)}]$ in (390) have the following large momentum asymptotics,

$$\lambda_{p,\mathrm{M}}[S^{(n)}] = 1 + O(p^{-2n})\,, \quad \mu_{p,\mathrm{M}}[S^{(n)}] = O(p^{-2n})\,. \tag{418}$$

Now suppose that $\omega_{H,2}$ be the two-point function of some Hadamard state. By (403)

$$\begin{aligned}\mathrm{WF}(\omega_2^{\mathrm{GSLE}}) &= \mathrm{WF}(\omega_2^{\mathrm{GSLE}} - \omega_{H,2} + \omega_{H,2}) \subseteq \mathrm{WF}(\omega_2^{\mathrm{GSLE}} - \omega_{H,2}) \cup \mathrm{WF}(\omega_{H,2})\\ &= \mathrm{WF}(\omega_2^{\mathrm{GSLE}} - \omega_{H,2}) \cup C^+\,,\end{aligned} \tag{419}$$

with C^+ defined in (401). Thus, to prove ω_2 is a Hadamard state, it is sufficient to show that $\mathrm{WF}(\omega_2 - \omega_{H,2}) = \emptyset$. To demonstrate this we shall need the following characterization of adiabatic vacua in terms of Sobolev wavefront sets from [56].

Lemma 5.6.3 (Lemma 3.3 from [56])**.**

Let $\omega_{H,2}$ and $\omega_{n,2}$ be the two-point functions of an arbitrary Hadamard state and the adiabatic vacuum of order $n \in \mathbb{N}_0$ (respectively) associated to the Klein-Gordon field on the four dimensional spacetime (M, g). Then

$$\forall\, s < 2n + \frac{3}{2} :\; WF^{\mathrm{s}}(\omega_{H,2} - \omega_{n,2}) = \emptyset\,. \tag{420}$$

Specializing henceforth to $d = 3$, fixing arbitrary $s \in \mathbb{R}$ and $n \in \mathbb{N}_0$ we have

$$\begin{aligned} \mathrm{WF}^s(\omega_2^{\mathrm{GSLE}} - \omega_{H,2}) &= \mathrm{WF}^s(\omega_2^{\mathrm{GSLE}} - \omega_{n,2} + \omega_{n,2} - \omega_{H,2}) \\ &\subseteq \mathrm{WF}^s(\omega_2^{\mathrm{GSLE}} - \omega_{n,2}) \cup \mathrm{WF}^s(\omega_{n,2} - \omega_{H,2})\,, \end{aligned} \tag{421}$$

and hence by Lemma 5.6.3

$$\forall\, s < 2n + \frac{3}{2} :\ \mathrm{WF}^s(\omega_2^{\mathrm{GSLE}} - \omega_{H,2}) \subseteq \mathrm{WF}^s(\omega_2^{\mathrm{GSLE}} - \omega_{n,2})\,. \tag{422}$$

We shall now show that for every $s \in \mathbb{R}$ it is possible to choose n sufficiently large so that the RHS of (422) is empty. This together with (409) above establishes that $\mathrm{WF}(\omega_2^{\mathrm{GSLE}} - \omega_{H,2}) = \emptyset$.

Consider the (formal) kernel of $\omega_2^{\mathrm{GSLE}} - \omega_{n,2}$,

$$\Delta W^{(n)}(\tau, x; \tau', x') := \int \frac{d^3p}{(2\pi)^3}\, e^{ip(x-x')}[T_{p,m,\mathrm{M}}(\tau)T_{p,m,\mathrm{M}}(\tau')^* - S^{(n)}_{p,\mathrm{M}=m}(\tau)S^{(n)}_{p,\mathrm{M}=m}(\tau')^*]\,. \tag{423}$$

Writing $T_{p,m,\mathrm{M}}(\tau) = S^{(n)}_{p,\mathrm{M}=m}(\tau) + \delta_{p,m,\mathrm{M}}(\tau)$, the estimates (417) and (418) imply $T_{p,m,\mathrm{M}} = S^{(n)}_{p,\mathrm{M}=m} + O(p^{-2n-\frac{1}{2}})$ and hence

$$T_{p,m,\mu}(t)T_{p,m,\mu}(t')^* - S^{(n)}_{p,\mu=m}(t)S^{(n)}_{p,\mu=m}(t')^* \;=\; O(p^{-2n-\frac{1}{2}})\,. \tag{424}$$

Moreover, as long as $m^2 > 0$ the integrand of (423) is continuous at the origin (as follows from an analysis of the small p behavior of the GSLE analogous to that in Section 5.3, thereby bridging a gap in the proof of [80]). Thus (424) entails that $\Delta W^{(n)}(\tau, x; \tau', x')$ is bounded by an absolutely convergent integral for all sufficiently large n, specifically for all points $(\tau, x), (\tau', x') \in M$

$$\forall\, n > \frac{5}{4} :\ \Delta W^{(n)}(\tau, x; \tau', x') \in \mathbb{C}\,. \tag{425}$$

Having proven that $\Delta W^{(n)}$ is a bi-*function*, we now prove that it is continuously differentiable. Consider a multi-index α and the mixed derivative $\partial^\alpha_{(y,y')}\Delta W^{(n)}(y, y')$. Pushing the derivative inside the integral in (423), we may bound this by an estimate on

$$\int \frac{d^3p}{(2\pi)^3}\, \partial^\alpha_{(x,x')} e^{ip(x-x')} \partial^\alpha_{(\tau,\tau')}[T_{p,m,\mathrm{M}}(\tau)T_{p,m,\mathrm{M}}(\tau')^* - S^{(n)}_{p,\mathrm{M}=m}(\tau)S^{(n)}_{p,\mathrm{M}=m}(\tau')^*]\,, \tag{426}$$

where clearly $\partial^\alpha_{(x,x')} e^{ip(x-x')} = O(p^{|\alpha|})$. It follows once more from (417) and (418) that $\partial^j_\tau \delta_{p,m,\mathrm{M}}(\tau) = O(p^{j-2n-1/2})$, and hence

$$\begin{aligned}
&\partial^\alpha_{(\tau,\tau')}[T_{p,m,\mathrm{M}}(\tau)T_{p,m,\mathrm{M}}(\tau')^* - S^{(n)}_{p,\mathrm{M}=m}(\tau)S^{(n)}_{p,\mathrm{M}=m}(\tau')^*] \\
&= \partial^\alpha_{(\tau,\tau')}[\delta_{p,m,\mathrm{M}}(\tau)S^{(n)}_{p,\mathrm{M}=m}(\tau')^* + S^{(n)}_{p,\mathrm{M}=m}(\tau)\delta_{p,m,\mathrm{M}}(\tau')^* + \delta_{p,m,\mathrm{M}}(\tau)\delta_{p,m,\mathrm{M}}(\tau')^*] \\
&= O(p^{|\alpha|-2n-1})\,. \qquad (427)
\end{aligned}$$

This yields the estimate

$$\begin{aligned}
&\left| \int \frac{d^3p}{(2\pi)^3}\, \partial^\alpha_{(x,x')} e^{ip(x-x')} \partial^\alpha_{(\tau,\tau')}[T_{p,m,\mathrm{M}}(\tau)T_{p,m,\mathrm{M}}(\tau')^* - S^{(n)}_{p,\mathrm{M}=m}(\tau)S^{(n)}_{p,\mathrm{M}=m}(\tau')^*] \right| \\
\leq\ & \text{const.} \int_0^\infty dp\, p^2 (1+p)^{|\alpha|-2n-1}\,, \qquad (428)
\end{aligned}$$

and thus the integral is absolute convergent as long as $|\alpha| \leq j(n) := 2n-3$.

Finally, since the action of the derivative $\partial^\alpha_{(y,y')}$ under the integral in (423) is integrable for $|\alpha| \leq j(n)$, it follows that $\Delta W^{(n)} \in C^{j(n)}(M \times M)$, and so it follows from (407) that $\Delta W^{(n)} \in H^{j(n)-3/2}_{\mathrm{loc}}(M)$. Hence we have proven that for any $s \in \mathbb{R}$, and for every $n \in \mathbb{N}_0$ with

$$s < 2n - 9/2 : \ \omega_2^{\mathrm{GSLE}} - \omega_{n,2} = \Delta W^{(n)} \in H^s_{\mathrm{loc}}(M \times M)\,. \qquad (429)$$

Equivalently, for every $s \in \mathbb{R}$ there exists an adiabatic order $n \in \mathbb{N}_0$ such that $\mathrm{WF}^s(\omega_2^{\mathrm{GSLE}} - \omega_{n,2}) = \emptyset$. Combined with (422) this entails

$$\forall\, s \in \mathbb{R} : \ \mathrm{WF}^s(\omega_2^{\mathrm{GSLE}} - \omega_{H,2}) = \emptyset\,. \qquad (430)$$

Finally, we recall (409)

$$\mathrm{WF}(\omega_2^{\mathrm{GSLE}} - \omega_{H,2}) = \overline{\bigcup_{s\in\mathbb{R}} \mathrm{WF}^s(\omega_2^{\mathrm{GSLE}} - \omega_{H,2})} = \emptyset\,, \qquad (431)$$

which completes the proof that the GSLE ω_2 is a Hadamard state.

□

5.7 Conclusions

The States of Low Energy (SLE) were introduced as Hadamard states [80] on generic Friedmann-Lemaître spacetimes with a physically appealing defining property. Here we showed that SLE have several bonus properties which make them mathematically and physically even more attractive. These bonus properties (a) – (e) have been listed in the introduction and need not be repeated here. Instead, we comment on some extensions and future directions.

As seen, the minimization over initial data results in an instructive alternative expression for the SLE solution solely in terms of the commutator function. A minimization over boundary data would likewise be relevant and occurs naturally when placing the basic wave equation into the setting of a regular Sturm-Liouville problem. Taking advantage of the literature on non-regular Sturm-Liouville problems might allow one to extend the SLE construction systematically to situations where the coefficient functions become singular within the interval considered. Covering the big bang singularity is of prime interest, but other singular points may be worthwhile treating as well, as the model from Section 5.5 illustrates.

The computation of the power spectrum requires access to the cross-over regime in the (time, momentum) plane. Ideally, one would be able to treat also the cross-over regime analytically by a suitable expansion. For physical reasons one would want to treat fully realistic cosmic evolutions where a pre-inflationary SLE replaces the positive frequency Hankel functions [86, 25, 71] and to propagate the resulting primordial power spectrum to the actual CMB.

Finally, our construction of the Generalized States of Low Energy shows explicitly that energy minimization, while physically appealing, is not at the mathematical core of obtaining a Hadamard state. One use of the GSLE we envision is in the context of the FLFRG, where the Hessian $\Gamma_k^{(2)}[\phi] - \mathcal{R}_k$ is field dependent. Constructing the inverse as a SLE via some fiducial solution S would entail a technically cumbersome field dependence of the Bogoliubov coefficients in (223), while in the GSLE construction the auxiliary scale M may be identified with the FRG flow parameter k, leaving the Bogoliubov coefficients in (388) independent of ϕ.

6.0 The Spatial FRG on Friedmann-Lemaître Spacetimes

6.1 Introduction

The Functional Renormalization Group (FRG) is a widely used reformulation of quantum field theory (QFT) in the spirit of the Wilsonian Renormalization Group. Favored for its ability to go beyond the weak-coupling expansions of standard perturbation theory, it has found application in areas diverse as solid-state physics, particle physics, and quantum gravity. The central objects of study in the FRG are one-parameter families of QFT functionals, whose behavior is captured in the form of functional integro-differential flow equations. Thus, the usual QFT problem of evaluating the functional integral for some bare action (435) is replaced with integrating these flow equations. We refer to [63, 104, 82, 30, 74, 102] for a systematic exposition of its standard formulation in Euclidean signature, focusing in this chapter on its formulation in Lorentzian Friedmann-Lemaître spacetimes.

For generality of presentation, we adopt the background field formalism on a generic Friedmann-Lemaître background with line element $ds^2 = \epsilon_g N(t)^2 dt^2 + a(t)^2 \delta_{ij} dx^i dx^j$. Both metric signatures are treated in parallel using $\epsilon_g = \pm 1$, highlighting the difference between a geometrically meaningful "Wick flip" ($\epsilon_g \mapsto -\epsilon_g$) and a pathological "Wick rotation" ($t \mapsto -it$) that complexifies the line element, with conventions

$$\begin{aligned} &\text{Euclidean:} \quad \epsilon_g = 1\,, \quad \sqrt{\epsilon_g} = 1\,, \\ &\text{Lorentzian:} \quad \epsilon_g = -1\,, \quad \sqrt{\epsilon_g} = i\,. \end{aligned} \tag{432}$$

A meaningful notion of a Wick rotation on a generic globally hyperbolic manifold would have to meet a number of desiderata, see e.g. [6]. Any known notion fails to meet one or more of these criteria. In contrast, the Wick flip is a weaker notion that simply maps a given Lorentzian manifold onto a Riemannian one, with no claims to analyticity or bijectivity.

To fix ideas, our starting point is the action $S + S_{\text{grav}}$ in $D = 1 + d$ dimensions

$$S[\tilde{\chi}; g] \;=\; \epsilon_g \int d^D y \sqrt{\epsilon_g g} \Big\{ \frac{1}{2} g^{\mu\nu} \partial_\mu \tilde{\chi} \partial_\nu \tilde{\chi} + \xi(\tilde{\chi}) R(g) + U(\tilde{\chi}) \Big\}$$

$$S_{\rm grav}[g] \;=\; \epsilon_g \int d^D y \sqrt{\epsilon_g g} \Big\{ \frac{1}{2\kappa}\big(2\Lambda_{\rm cosm} - R\big) + \frac{1}{2s}\mathcal{C}^2 + \omega_0 R^2 - \frac{\theta}{s}\mathcal{G} \Big\}\,, \tag{433}$$

where the inclusion of general even potentials U, ξ in the matter action is motivated by the Wilsonian framework. The fourth order gravity action is conveniently parameterized in terms of the Weyl tensor squared $\mathcal{C}^2$ and the Gauss-Bonnet term $\mathcal{G}$. We note, however, that for a $1+3$ dimensional Friedmann-Lemaître cosmology $\mathcal{C}^2 = 0$ and $\mathcal{G}$ is a total derivative.

Expanding the matter action around a background field $\phi(t,x)$, the one-parameter family of functionals is then defined via the introduction of a term ΔS_k that modulates the fluctuation field χ,

$$S_k[\chi; g, \phi] = S[\phi + \chi; g] + \Delta S_k[\chi; g]\,, \quad \Delta S_k[\chi; g] = \frac{\epsilon_g}{2}\chi \cdot \mathcal{R}_k \cdot \chi\,, \tag{434}$$

where as usual the "$\cdot$" represents an integration with respect to the standard (pseudo) Riemannian volume density. The regulator kernel $\mathcal{R}_k$ is taken to modulate the eigenvalues of the full Laplacian ∇^2 in Euclidean signature, or those of the spatial Laplacian ∇_s^2 in Lorentzian signature. In the Riemannian setting, the ellipticity of ∇^2 enables discrimination between large and small momentum modes (where by "large/small" we refer to the individual momentum components) by the corresponding eigenvalues of ∇^2. Hence, modulating the mode content according to the eigenvalues of ∇^2 leads to a well defined *covariant* coarse-graining procedure. On the other hand, the existence of null-momenta in a Lorentzian spacetime renders such an identification untenable, excepting a Wick rotation. However, since a sufficiently general notion of a Wick rotation is unavailable for generic Friedmann-Lemaître backgrounds [6], the route pursued here is to replace the covariant modulation with a merely spatial one through $\mathcal{R}_k(t,x;t',x') = \delta(t,t')R_k(t,x;t,x')$, while leaving the temporal dynamics unaffected. Moreover, the kernel R_k modulates only the spatial modes according to the eigenvalues of the spatial Laplacian ∇_s^2, yielding a well defined form of mode-blocking. In terms of a spectral representation in the Lorentzian setting, the regulator kernel $R_k(t,p^2)$ is required to satisfy the following general properties (see Appendix E of [89] for the Euclidean case)

Reg (i) $R_k(t,p^2) \to 0$ for $k \to 0$, ensuring that the $k \to 0$ limit of the various functionals coincide with their usual definitions.

Reg (ii) $R_k(t,p^2) \sim k^2$ for $p^2 \lesssim k^2$, giving an effective $O(k^2)$ mass to the slow-modes.

Reg (iii) $R_k(t,p^2)$ approaches zero sufficiently fast for $p^2 \gg k^2$, thereby leaving the fast-modes to be integrated out in the functional integral without a suppression factor.

Having introduced the mode modulation, the background field generating functional $W_k[J;\phi]$ and effective average action $\Gamma_k[\varphi;\phi]$ are defined as usual,

$$e^{\frac{1}{\sqrt{\epsilon_g}\hbar}W_k[J;\phi]} = \int \mathcal{D}\chi\, e^{-\frac{1}{\sqrt{\epsilon_g}\hbar}(S[\phi+\chi]+\Delta S_k[\chi])+\frac{1}{\sqrt{\epsilon_g}\hbar}J\cdot\chi}, \tag{435}$$

$$\Gamma_k[\varphi;\phi] = J_k[\varphi;\phi]\cdot\varphi - W_k\big|_{J=J_k[\varphi;\phi]} - \Delta S_k[\varphi]\,, \quad \frac{\delta W_k}{\delta J}\Big|_{J=J_k[\varphi;\phi]} \stackrel{!}{=} \varphi\,. \tag{436}$$

In general the regulator $\mathcal{R}_k$ may depend on the background field ϕ, in which case the action (434) depends the fluctuation field and the background field *separately*, i.e. not just through their sum. On the level of the effective action (436) this means that the *splitting symmetry* $\Gamma_k[\varphi+\zeta;\phi-\zeta] = \Gamma_k[\varphi;\phi]$ is violated. However, it is readily verified that as long as $\mathcal{R}_k$ is independent of the background field ϕ that splitting symmetry is maintained, i.e. $\Gamma_k[\varphi;\phi] = \Gamma_k[\varphi+\phi]$ (by slight abuse of notation)[1].

Differentiating $W_k[J;\phi]$ with respect to k yields the familiar Polchinski equation

$$k\partial_k W_k[J;\phi] = -\frac{\epsilon_g}{2}\mathrm{Tr}\left\{k\partial_k\mathcal{R}_k\left[\frac{\delta W_k}{\delta J}\frac{\delta W_k}{\delta J} + \sqrt{\epsilon_g}\hbar\frac{\delta^2 W_k}{\delta J\delta J}\right]\right\}, \tag{437}$$

where we note that the trace over spacetime indices is with respect to the usual volume density. Implementing the modified Legendre transformation in (436),

$$\begin{aligned} k\partial_k\Gamma_k[\varphi;\phi] &= k\partial_k J_k[\varphi;\phi]\cdot\varphi - k\partial_k J_k[\varphi;\phi]\cdot\frac{\delta W_k}{\delta J}\Big|_{J=J_k} - k\partial_k W_k\big|_{J=J_k} - k\partial_k\Delta S_k[\varphi] \\ &= -k\partial_k W_k\big|_{J=J_k} - \frac{\epsilon_g}{2}\mathrm{Tr}\left\{k\partial_k\mathcal{R}_k\frac{\delta W_k}{\delta J}\frac{\delta W_k}{\delta J}\right\} \\ &= \frac{\epsilon_g\sqrt{\epsilon_g}\hbar}{2}\mathrm{Tr}\left\{k\partial_k\mathcal{R}_k\frac{\delta^2 W_k}{\delta J\delta J}\Big|_{J=J_k[\varphi;\phi]}\right\}. \end{aligned} \tag{438}$$

[1] In the context of quantum gravity, the regulator typically depends on the background metric $\bar{g}$, breaking splitting symmetry. However, a Ward identity for splitting symmetry holds, see Section 2.4 of [89].

Moreover, it follows from the definition of the (modified) Legendre transformation that

$$\frac{\delta^2 W_k}{\delta J \delta J}\Big|_{J=J_k[\varphi;\phi]} = \left[\frac{\delta^2 \Gamma_k}{\delta\varphi\delta\varphi} + \epsilon_g \mathcal{R}_k\right]^{-1} . \tag{439}$$

For our purposes a background independent $\mathcal{R}_k$ suffices and we can set the mean field φ to zero, writing $\Gamma_k[\phi] = \Gamma_k[0;\phi]$. Further, splitting symmetry entails $\frac{\delta^2\Gamma_k}{\delta\varphi\delta\varphi} = \frac{\delta^2\Gamma_k}{\delta\phi\delta\phi}$, yielding the Wetterich equation

$$k\partial_k \Gamma_k[\phi] \;=\; \frac{\epsilon_g\sqrt{\epsilon_g}\hbar}{2}\mathrm{Tr}\big\{k\partial_k\mathcal{R}_k\, G_k[\phi]\big\}\,, \quad \left[\frac{\delta^2\Gamma_k}{\delta\phi\delta\phi} + \epsilon_g\mathcal{R}_k\right]\cdot G_k[\phi] = \mathbb{1}\,. \tag{440}$$

Motivated by the role of the one-loop effective action in setting the UV boundary data for the (otherwise kinematical) Wetterich equation (see Figure 2), as well as the recent interest in the recovery of perturbative results from the FRG [22], we shall use (440) to renormalize the more general action (441) to one-loop order on a generic Friedmann-Lemaître background, highlighting key differences to the standard covariant computation.

6.2 One-loop effective action on Friedmann-Lemaître spacetimes

Adopting a Wilsonian standpoint, in this section we consider the one-loop renormalization for a scalar theory with general even potential $U(\tilde{\chi})$ on a Lorentzian Friedmann-Lemaître background in $d = 3$ spatial dimensions. As we shall discover, this generically necessitates the inclusion of non-minimal gravity couplings to all orders, specifically we generalize our bare action from the fourth order gravity action of (433) to

$$S[\tilde{\chi};g] \;=\; -\int d^4y\sqrt{-g}\Big\{\frac{1}{2}g^{\mu\nu}\partial_\mu\tilde{\chi}\partial_\nu\tilde{\chi} + \sum_{n\geq 0}\,{}^nU(\tilde{\chi})R^n\Big\}\,, \tag{441}$$

with even (bare) potentials

$${}^nU(\tilde{\chi}) = \sum_{j\geq 0}\frac{1}{(2j)!}\,{}^nu_{2j}\tilde{\chi}^{2j}\,, \quad n\geq 0\,. \tag{442}$$

Note that ${}^nu_{2j}$ has mass dimension $4-2(j+n)$, and hence for any $N\in\mathbb{N}_0$ there are $N+1$ couplings of mass dimension $4-2N$. In particular, only the ones with $N = 0,1,2$ have

non-negative mass dimension, which are

$$
\begin{aligned}
{}^0u_0 &= \frac{\Lambda_{\rm cosm}}{\kappa}\,, \qquad {}^0u_2 = m^2\,, \qquad {}^0u_4 = \lambda\,,\\
{}^1u_0 &= -\frac{1}{\kappa}\,, \qquad {}^1u_2 = \xi\,,\\
{}^2u_0 &= \omega_0\,,
\end{aligned}
\tag{443}
$$

where we have indicated the conventional notation, see (433).

Next, we introduce the general structure of the counterterm Lagrangian. Throughout we denote bare quantities (diverging as $\Lambda \to \infty$) by a subscript Λ while renormalized quantities carry no subscript but tacitly refer to a finite renormalization scale μ. Both are as usual related by a renormalization constant where the subscript Λ is omitted. Writing

$$
-L_\Lambda = -\frac{1}{2}\phi_\Lambda \nabla^2 \phi_\Lambda + \sum_{n\geq 0} {}^nU_\Lambda(\phi_\Lambda) R^n\,,
\tag{444}
$$

the bare field ϕ_Λ is related to the renormalized one ϕ by $\phi_\Lambda = Z^{1/2}\phi$. The bare potentials ${}^nU_\Lambda(\phi_\Lambda)$ then expand according to

$$
\begin{aligned}
{}^nU_\Lambda(\phi_\Lambda) &= \sum_{j\geq 0} \frac{1}{(2j)!}\, {}^nu_{2j,\Lambda}\phi_\Lambda^{2j} = \sum_{j\geq 0} \frac{1}{(2j)!}\, {}^nZ_{2j}\, {}^nu_{2j}\phi^{2j}\,,\\
Z^j\, {}^nu_{2n,\Lambda} &= {}^nZ_{2j}\, {}^nu_{2j}\,, \quad n\geq 0\,,\, j\geq 0\,,
\end{aligned}
\tag{445}
$$

where all the renormalization constants are $1 + O(\hbar)$, and hence $L_\Lambda = L + \hbar L_{\rm ct}$.

6.2.1 Identifying the ultraviolet divergences

We shall use the Wetterich equation (440) to isolate the UV-divergent contributions to the effective action associated to (441). Proceeding manifestly in Lorentzian signature with line element $ds^2 = -N(t)^2dt^2 + a(t)^2\delta_{ij}dx^idx^j$, the regulator $\mathcal{R}_k(t,x;t',x') = \delta(t,t')R_k(t,x;t,x')$[2] now modulates only spatial modes. In a spatial momentum space representation the kernel is

$$
R_k(t,x;t,x') \;=\; \int \frac{d^3p}{(2\pi)^3}\, e^{ip(x-x')} R_k(t,p^2)\,, \quad R_k(t,p^2) = k^2 r(\tfrac{p^2}{a(t)^2k^2})\,,
\tag{446}
$$

[2]The temporal delta function is normalized $\delta(t,t') = N(t)a(t)^d\delta(t-t')$.

with the time dependence entering through the "physical momentum" $p^2/a(t)^2$. Inserting the $\hbar$-expansion $\Gamma_k[\phi] = \Gamma_{k,0}[\phi] + \sum_{n\geq 1} \hbar^n \Gamma_{k,n}[\phi]$ into the Wetterich equation readily yields that $\Gamma_{k,0}[\phi] \equiv \Gamma_0[\phi]$ is k-independent. It follows from a saddle-point evaluation of the functional integral that $\Gamma_0[\phi]$ coincides with the "renormalized action" $S = \int d\mathrm{vol}(g) L$,

$$\Gamma_{k,0}[\phi] \;\equiv\; \Gamma_0[\phi] \;=\; S[\phi]\,. \tag{447}$$

In turn, the S determines the k-flow of the one-loop correction $\Gamma_{k,1}$,

$$k\partial_k \Gamma_{k,1}[\phi] \;=\; -\frac{i}{2}\mathrm{Tr}\big\{k\partial_k \mathcal{R}_k G_k[\phi]\big\}\,, \quad \big[S^{(2)}[\phi] - \mathcal{R}_k\big]\cdot G_k[\phi] = \mathbb{1}\,. \tag{448}$$

Specializing to conformal time gauge $N(\eta) = a(\eta)$, and restricting to spatially homogeneous mean fields $\phi(\eta)$, this reads

$$k\partial_k \Gamma_{k,1}[\phi] \;=\; -\frac{i}{2}\int d\eta d^3x\, a(\eta)^4 \int \frac{d^3p}{(2\pi)^3} k\partial_k R_k(\eta,p) G_k(\eta,p)\,. \tag{449}$$

By slight abuse of notation we write $G_k(\eta,p)$ for the temporal coincidence limit of the Fourier transformed green function $G_k(\eta,\eta';p)$, which satisfies

$$\big[a^{-4}\partial_\eta(a^2\partial_\eta) + a^{-2}p^2 + R_k(\eta,p) + V(\eta)\big] G_k(\eta,\eta';p) = -\delta(\eta,\eta')\,, \tag{450}$$

where we have defined the "potential"

$$V(\eta) := \sum_{n\geq 0} {}^nU''(\phi(\eta)) R(\eta)^n\,. \tag{451}$$

Recalling the covariant normalization of $\delta(\eta,\eta') = a(\eta)^{-4}\delta(\eta-\eta')$, the first order term may be removed by defining $\mathcal{G}_k(\eta,\eta';p) := a(\eta)a(\eta')G_k(\eta,\eta';p)$. This yields

$$\big[\partial_\eta^2 + p^2 + a(\eta)^2 R_k(\eta,p) + a(\eta)^2(V(\eta) - R(\eta)/6)\big]\mathcal{G}_k(\eta,\eta';p) = -\delta(\eta-\eta')\,, \tag{452}$$

together with the corresponding flow equation

$$k\partial_k \Gamma_{k,1}[\phi] \;=\; -\frac{i}{2}\int d\eta d^3x \int \frac{d^3p}{(2\pi)^3} k\partial_k(a^2 R_k)(\eta,p)\mathcal{G}_k(\eta,p)\,. \tag{453}$$

The computation of the full one-loop correction to the effective action

$$\Gamma_{0,1}[\phi] \;=\; \Gamma_{\Lambda,1}[\phi] - \int_0^\Lambda dk\, \partial_k \Gamma_{k,1}[\phi] \tag{454}$$

then requires specification of the Green function $\mathcal{G}_k(\eta,\eta';p)$ satisfying (452) for all $k \in (0,\Lambda)$. It is clear from (452) that such a specification is analogous to choice of vacuum state for a free QFT on the Friedmann-Lemaître background, and is hence highly non-unique. Thus, unlike the standard Euclidean FRG where ellipticity of the Hessian $\Gamma_k^{(2)} + \mathcal{R}_k$ entails a unique Green function, the spatial formulation necessitates the incorporation of state-dependent aspects into the flow equation, which will impact the flow pattern for small k (see Figure 2). However, in order to identify the one-loop counterterms $\Gamma_{\Lambda,1}[\phi]$ required to render the (454) UV-finite, only universal state-independent information enters. Specifically, splitting the integral (454) according to

$$\Gamma_{0,1}[\phi] \;=\; \Gamma_{\Lambda,1}[\phi] - \int_\mu^\Lambda dk\, \partial_k \Gamma_{k,1}[\phi] - \int_0^\mu dk\, \partial_k \Gamma_{k,1}[\phi]\,, \tag{455}$$

it is sufficient to study the flow of (453) for $\Lambda \geq k \geq \mu$ with μ sufficiently large. The form of $\mathcal{G}_k(\eta,p)$ in this regime is determined by the generalized resolvent expansion, presented in Section 5.4.2. This is implemented by first rescaling $p = k\wp$ in (452), (453), and then taking k to be large, with the Gelfand-Dickey equation (326) for $\mathcal{G}_k(\eta,\wp) := \mathcal{G}_k(\eta,p)|_{p=k\wp}$ reading

$$2\mathcal{G}_k(\eta,\wp)\partial_\eta^2 \mathcal{G}_k(\eta,\wp) - (\partial_\eta \mathcal{G}_k(\eta,\wp))^2 + 4\big[k^2\omega_2(\eta,\wp)^2 + \omega_0(\eta)^2\big]\mathcal{G}_k(\eta,\wp)^2 = -1\,, \tag{456}$$

$$\omega_2(\eta,\wp)^2 := \wp^2 + a(\eta)^2 r(\tfrac{\wp^2}{a(\eta)^2})\,, \quad \omega_0(\eta)^2 := a(\eta)^2\big[V(\eta) - R(\eta)/6\big]\,,$$

and the flow equation

$$\partial_k \Gamma_{k,1}[\phi] \;=\; -\frac{8ik^4}{(4\pi)^2}\int d\eta d^3x \int_0^\infty d\wp\, \wp^2\big[r(\wp^2/a^2) - \wp^2/a^2 r'(\wp^2/a^2)\big]\mathcal{G}_k(\eta,\wp)\,. \tag{457}$$

Inserting the large k expansion

$$\mathcal{G}_k(\eta,\wp) \asymp -\frac{i}{2\omega_2(\eta,\wp)k}[1 + \sum_{n\geq 1}(-)^n \bar{G}_n(\eta,\wp)k^{-2n}] \tag{458}$$

converts (456) into the recursion (cf. (328) from Section 5.4.2)

$$\bar{G}_n = \sum_{j,l\geq 0, j+l=n-1} \Big\{ \frac{1}{4}\frac{\bar{G}_k}{\omega_2}\partial_\eta^2\Big(\frac{\bar{G}_l}{\omega_2}\Big) - \frac{1}{8}\partial_\eta\Big(\frac{\bar{G}_k}{\omega_2}\Big)\partial_\eta\Big(\frac{\bar{G}_l}{\omega_2}\Big) + \frac{1}{2}\frac{\omega_0^2}{\omega_2^2}\bar{G}_j\bar{G}_l\Big\} - \frac{1}{2}\sum_{j,l\geq 1, j+l=n} \bar{G}_j\bar{G}_l. \tag{459}$$

Thus $\bar{G}_n$ may be expressed in terms of $\bar{G}_{n-1},\ldots,\bar{G}_1$, and involves only differentiations. It follows that all $\bar{G}_n$ are differential polynomials in $v := \omega_0^2, w := \omega_2^2$. Moreover, by inserting the resolvent expansion (458) into the flow equation (457) and performing the large-k integral (455), it follows that only $\bar{G}_1, \bar{G}_2$ contribute to the UV-divergences. We recall from (329) their explicit expressions

$$\begin{aligned}
\bar{G}_1 &= \frac{v}{2w} + \frac{5}{32}\frac{w'^2}{w^3} - \frac{1}{8}\frac{w''}{w^2}\,, \\
\bar{G}_2 &= \frac{3}{8w^2}\Big(v^2 + \frac{1}{3}v''\Big) - \frac{5}{16w^3}\Big(vw'' + v'w' - v\frac{7w'^2}{4w}\Big) \\
&+ \frac{1}{32w^3}\Big(-w^{(4)} + \frac{21w''^2}{4w} + \frac{7w^{(3)}w'}{w} - \frac{231w'^2w''}{8w^2} + \frac{1155w'^4}{64w^3}\Big)\,,
\end{aligned} \tag{460}$$

where we momentarily denote ∂_η differentiations with a "$'$" for brevity. The flow equation of the UV-divergent part $\Gamma_{k,1}^{\rm div}$ of $\Gamma_{k,1}$ is

$$\partial_k\Gamma_{k,1}^{\rm div}[\phi] \;=\; -\frac{4k^3}{(4\pi)^2}\int d\eta d^3x\, a(\eta)^4 \int_0^\infty d\varrho\, \varrho^2 \frac{[r(\varrho^2) - \varrho^2 r'(\varrho^2)]}{[\varrho^2 + r(\varrho^2)]^{1/2}}\Big\{1 - \frac{G_1(\eta,\varrho)}{k^2} + \frac{G_2(\eta,\varrho)}{k^4}\Big\}\,, \tag{461}$$

where we have redefined $\wp = a(\eta)\varrho$ and $G_j(\eta,\varrho) := \bar{G}_j(\eta,\wp)|_{\wp=a(\eta)\varrho}$[3]. Upon insertion into (455), evaluating $-\int_\mu^\Lambda dk\,\partial_k\Gamma_{k,1}^{\rm div}[\phi]$ yields the UV-divergent contribution to the one-loop correction,

$$\Gamma_1^{\rm div}[\phi] \;=\; \frac{1}{(4\pi)^2}\int d\eta dx\, a(\eta)^4\Big\{q_0(\Lambda^4 - \mu^4) + g_1(\eta)(\Lambda^2 - \mu^2) + g_2(\eta)\ln(\Lambda/\mu)\Big\}\,, \tag{462}$$

where we have kept the terms from the lower integration boundary to maintain $\Gamma_1^{\rm div}[\phi]|_{\Lambda=\mu} =$

[3]It is to be understood that the redefinition $\wp = a(\eta)\varrho$ is to be performed *after* all the time derivatives in (460) have been performed.

0. Further

$$
\begin{aligned}
q_0 &= \int_0^\infty d\varrho\, \varrho^2 \frac{[r(\varrho^2) - \varrho^2 r'(\varrho^2)]}{[\varrho^2 + r(\varrho^2)]^{1/2}}\,, \\
g_1(\eta) &= -2\int_0^\infty d\varrho\, \varrho^2 \frac{[r(\varrho^2) - \varrho^2 r'(\varrho^2)]}{[\varrho^2 + r(\varrho^2)]^{1/2}} G_1(\eta,\varrho)\,, \\
g_2(\eta) &= 4\int_0^\infty d\varrho\, \varrho^2 \frac{[r(\varrho^2) - \varrho^2 r'(\varrho^2)]}{[\varrho^2 + r(\varrho^2)]^{1/2}} G_2(\eta,\varrho)\,,
\end{aligned} \tag{463}
$$

The expressions for $g_1(\eta)$ and $g_2(\eta)$

$$
\begin{aligned}
g_1(\eta) &= q_{1,1} R + q_{1,2}(V - R/6) \\
g_2(\eta) &= \frac{1}{2}(V - R/6)^2 - \frac{1}{6}\nabla^2(V - R/6) \\
&+ B_1 \frac{a^{(4)}}{a^5} + B_2 \frac{a^{(1)} a^{(3)}}{a^6} + B_3 \frac{a^{(2)\,2}}{a^6} + B_4 \frac{a^{(1)\,2} a^{(2)}}{a^7} + B_5 \frac{a^{(1)\,4}}{a^8} \\
&+ \Big(B_6 \frac{R}{6} + B_7 \frac{a^{(1)\,2}}{a^4} \Big)(V - R/6) + B_8 \frac{a^{(1)}}{a^3} \partial_\eta (V - R/6)\,,
\end{aligned} \tag{464}
$$

carry a dependence on the regulator $r(x)$ arising from the ϱ-integrals in (463), which is contained in the coefficients $q_{1,1}, q_{1,2}, B_j$. We have also left the η dependencies implicit, and denote by $a^{(n)} := \partial_\eta^n a$.

As may be expected from our use of a *non-covariant spatial regulator*, the structure of the logarithmic divergence from the second and third lines of $g_2(\eta)$ above has a non-covariant form. Remarkably, it follows from the properties of the regulator function (**Reg(i)-(iii)** in Section 6.1) that $g_2(\eta)$ can be "covariantized" and expressed

$$
R = \frac{6a^{(2)}}{a^3}\,, \quad \nabla^2 R = -6\frac{a^{(4)}}{a^5} + 24\frac{a^{(1)} a^{(3)}}{a^6} + 18\frac{a^{(2)\,2}}{a^6} - 36\frac{a^{(1)\,2} a^{(2)}}{a^7} \tag{465}
$$

$$
-R_{\mu\nu}R^{\mu\nu} + \frac{1}{3}R^2 = -12\frac{a^{(1)\,4}}{a^8} + 12\frac{a^{(1)\,2} a^{(2)}}{a^7} = \frac{4}{a^4}\partial_\eta\Big(\frac{a^{(1)\,3}}{a^3}\Big)\,, \tag{466}
$$

for generic regulator functions $r(x)$. This is the content of the following lemma.

Lemma 6.2.1.

Let $r(x)$ be a generic FRG regulator function as defined in (446).

(i) The regulator dependent coefficients B_1, B_2, B_3 always satisfy the ratio

$$B_1 : B_2 : B_3 \;=\; -1 : 4 : 3\,, \tag{467}$$

and hence can be expressed in terms of a single regulator dependent constant $q_{0,1}$,

$$B_1 = -6q_{0,1}\,, \quad B_2 = 24q_{0,1}\,, \quad B_3 = 18q_{0,1}\,. \tag{468}$$

(ii) $B_4 + 36q_{0,1} + B_5 = 0$.

(iii) $B_6 = B_7 = B_8$.

The proof of Lemma 6.2.1, as well as explicit expressions for $q_{1,1}, q_{1,2}$ and $q_{0,1}, q_{0,2}, q_{0,3}$ (defined below) are relegated to Appendix B.

Next, it follows from the explicit expressions (465), (466) for the curvature invariants, together with Lemma 6.2.1(i), (ii) that

$$\begin{aligned}
&B_1\frac{a^{(4)}}{a^5} + B_2\frac{a^{(1)}a^{(3)}}{a^6} + B_3\frac{a^{(2)\,2}}{a^6} + B_4\frac{a^{(1)\,2}a^{(2)}}{a^7} + B_5\frac{a^{(1)\,4}}{a^8} \\
&= \; q_{0,1}\nabla^2 R + (B_4 + 36q_{0,1})\frac{a^{(1)\,2}a^{(2)}}{a^7} + B_5\frac{a^{(1)\,4}}{a^8} \\
&= \; q_{0,1}\nabla^2 R - \frac{B_5}{12}\Big[12\frac{a^{(1)\,2}a^{(2)}}{a^7} - 12\frac{a^{(1)\,4}}{a^8}\Big] \\
&= \; q_{0,1}\nabla^2 R + q_{0,2}\Big[- R_{\mu\nu}R^{\mu\nu} + \frac{1}{3}R^2\Big]\,.
\end{aligned} \tag{469}$$

Moreover, Lemma 6.2.1(iii) entails that the final line of $g_2(\eta)$ in (464) may be expressed in terms of a single coefficient $q_{0,3} := B_8$,

$$\Big(B_6\frac{R}{6} + B_7\frac{a^{(1)\,2}}{a^4}\Big)(V - R/6) + B_8\frac{a^{(1)}}{a^3}\partial_\eta(V - R/6) \;=\; q_{0,3}a^{-4}\partial_\eta\big[aa^{(1)}(V - R/6)\big]\,. \tag{470}$$

In summary g_1 and g_2 are expressible in terms of curvature invariants and total derivatives,

$$\begin{aligned}
g_1(\eta) \;&=\; q_{1,1}R + q_{1,2}(V - R/6)\,, \\
g_2(\eta) \;&=\; \frac{1}{2}(V - R/6)^2 - \frac{1}{6}\nabla^2(V - R/6) \\
&+\; q_{0,1}\nabla^2 R + q_{0,2}\Big[- R_{\mu\nu}R^{\mu\nu} + \frac{1}{3}R^2\Big] \\
&+\; q_{0,3}a^{-4}\partial_\eta\big[aa^{(1)}(V - R/6)\big]\,.
\end{aligned} \tag{471}$$

Finally, the second and third lines of $g_2(\eta)$ in (471) are a total derivative, which follows from the explicit expressions (465), (466). Hence upon $\int d\eta d^3x a(\eta)^4$ integration in (462) these evaluate to a boundary term, which may be omitted. Thus, up to boundary terms, the UV-divergent correction to the one-loop effective action is

$$\begin{aligned}\hbar\Gamma_1^{\rm div}[\phi] &= \int d\eta dx\, a^4 L_1^{\rm div} \\ L_1^{\rm div} &:= \frac{\hbar}{(4\pi)^2}\Big\{q_0(\Lambda^4-\mu^4)+\big[q_{1,1}R+q_{1,2}(V-R/6)\big](\Lambda^2-\mu^2) \\ &+ \frac{1}{2}(V-R/6)^2\ln(\Lambda/\mu)\Big\} \end{aligned} \tag{472}$$

with V from (451). We remark that this divergence structure is akin to that obtained in a covariant setting, up to an additional quadratic divergence proportional to $q_{1,1}R$ originating from the time dependence of the regulator $R_k(\eta,p)$. These divergences ought to be absorbed by counterterms in $\Gamma_{\Lambda,1}$. We anticipate that the novel $q_{1,1}$ term will lead to an additional renormalization of Newton's constant.

6.2.2 Renormalization study

We now examine the general structure of the counterterm Lagrangian. It is clear from (472) that the one-loop divergence structure does not necessitate a non-trivial wavefunction renormalization, i.e. $Z = 1 + O(\hbar^2)$. Thus the bare and renormalized couplings in (445) are related by

$${}^n u_{2n,\Lambda} = {}^n Z_{2j}\, {}^n u_{2j}\,, \quad n \geq 0\,,\, j \geq 0\,, \tag{473}$$

and we choose appropriate Ansätze for the renormalization constants:

$$\begin{aligned} {}^0Z_0 &= 1+\frac{\hbar}{(4\pi)^2}\Big\{\,{}^0z_{0,0}+\,{}^0z_{0,1}\ln\Lambda/\mu+\,{}^0z_{0,2}(\Lambda/\mu)^2+\,{}^0z_{0,4}(\Lambda/\mu)^4\Big\}\,, \\ {}^0Z_{2j} &= 1+\frac{\hbar}{(4\pi)^2}\Big\{\,{}^0z_{2j,0}+\,{}^0z_{2j,1}\ln\Lambda/\mu+\,{}^0z_{2j,2}(\Lambda/\mu)^2\Big\}\,, \quad j\geq 1\,, \\ {}^nZ_{2j} &= 1+\frac{\hbar}{(4\pi)^2}\Big\{\,{}^nz_{2j,0}+\,{}^nz_{2j,1}\ln\Lambda/\mu+\,{}^nz_{2j,2}(\Lambda/\mu)^2\Big\}\,, \quad n\geq 1,\, j\geq 0\,. \end{aligned} \tag{474}$$

In all cases $O(\hbar^2)$ corrections are implicit. The Ansätze (474) contain non-divergent terms, which are however related to the coefficients of the powerlike terms by the "matching principle" of [78]: we seek to identify the renormalized couplings with the bare ones at scale μ. This constrains the coefficients of the non-logarithmic terms as follows

$$
\begin{aligned}
&{}^0z_{0,0} + {}^0z_{0,2} + {}^0z_{0,4} = 0\,, \quad {}^0z_{2j,0} + {}^0z_{2j,2} = 0\,, \quad j \geq 1\,,\\
&{}^nz_{2j,0} + {}^nz_{2j,2} = 0\,, \quad n \geq 1,\, j \geq 0\,.
\end{aligned}
\tag{475}
$$

The counterterm action thus reads

$$
L_\Lambda = L - \frac{\hbar}{(4\pi)^2}\Big\{\mu^{-4}\,{}^0u_0\,{}^0z_{0,4}\,\Lambda^4 + F_2\,\Lambda^2 + F_4\ln(\Lambda/\mu) + O(\Lambda^0)\Big\}\,. \tag{476}
$$

Here

$$
\begin{aligned}
F_2 &= \mu^{-2}\sum_{n\geq 0}\sum_{j\geq 0}\frac{1}{(2j)!}\,{}^nz_{2j,2}\,{}^nu_{2j}\phi^{2j}R^n\,,\\
F_4 &= \sum_{n\geq 0}\sum_{j\geq 0}\frac{1}{(2j)!}\,{}^nz_{2j,1}\,{}^nu_{2j}\phi^{2j}R^n\,.
\end{aligned}
\tag{477}
$$

Then, the finiteness condition $L_\Lambda + L_1^{\rm div} =$ finite as $\Lambda \to \infty$ amounts to

$$
{}^0u_0\,{}^0z_{0,4} = \mu^4 q_0\,, \tag{478}
$$

$$
F_2 = q_{1,1}R + q_{1,2}(V - R/6)\,, \tag{479}
$$

$$
F_4 = \frac{1}{2}(V - R/6)^2\,. \tag{480}
$$

The occurrence of the $V - R/6$ in (479), (480) makes it convenient for notational purposes to define the potentials ${}^n\bar U(\phi)$ and couplings ${}^n\bar u_{2j}$,

$$
\begin{aligned}
{}^n\bar U(\phi) &= \sum_{n\geq 0}\sum_{j\geq 0}\frac{1}{(2j)!}\,{}^n\bar u_{2j}\phi^{2j}R^n\,,\\
{}^1\bar U(\phi) &:= {}^1U(\phi) - \frac{1}{12}\phi^2\,, \quad {}^n\bar U(\phi) := {}^nU(\phi)\,, \quad n \neq 1\,,\\
{}^1\bar u_2 &= {}^1u_2 - \frac{1}{6}\,, \quad {}^n\bar u_{2j} = {}^nu_{2j} \quad \text{else}\,.
\end{aligned}
\tag{481}
$$

Re-expressing (479), (480) in terms of these yields

$$F_2 \stackrel{!}{=} q_{1,2}\,{}^0\bar{U}''(\phi) + \big[q_{1,1} + q_{1,2}\,{}^1\bar{U}''(\phi)\big]R + q_{1,2}\sum_{n\geq 2}\,{}^n\bar{U}''(\phi)R^n \tag{482}$$

$$\begin{aligned} 2F_4 \stackrel{!}{=}\ & {}^0\bar{U}''(\phi)^2 + 2\,{}^0\bar{U}''(\phi)\,{}^1\bar{U}''(\phi)R + \big[2\,{}^0\bar{U}''(\phi)\,{}^2\bar{U}''(\phi) + {}^1\bar{U}''(\phi)^2\big]R^2 \\ & + \sum_{n\geq 3}\Big[\sum_{n_1+n_2=n}\,{}^{n_1}\bar{U}''(\phi)\,{}^{n_2}\bar{U}''(\phi)\Big]R^n\,. \end{aligned} \tag{483}$$

Before matching the coefficients of $\phi^{2j}R^n$ to obtain expressions for the renormalization constants ${}^nZ_{2j}$, and subsequently the beta functions, we add several remarks on the renormalization structure implied by (482), (483):

Remarks:

(i) The divergence structure of the pure scalar potential ${}^0U(\phi) \equiv {}^0\bar{U}(\phi)$ in $L_1^{\rm div}$

$$\frac{\hbar}{(4\pi)^2}\Big\{q_{1,2}\,{}^0U''(\phi)\Lambda^2 + \frac{1}{2}\,{}^0U''(\phi)^2\ln(\Lambda/\mu)\Big\}\,, \tag{484}$$

where we have omitted the cosmological constant term (478), is identical to that in flat spacetime. Thus the renormalization of the pure scalar couplings ${}^0u_{2j}$, detailed below, is unaffected by the higher order couplings to the Ricci scalar.

(ii) It follows from the F_2-relation (482) that as far as the quadratic divergence is concerned, the renormalized couplings ${}^nu_{2j}$ in the potential ${}^nU(\phi) = \sum_{j\geq 0}\frac{1}{(2j)!}\,{}^nu_{2j}\phi^{2j}$ affect *only* the renormalization constants ${}^nZ_{2j}$, i.e. there is no mixing in the Ricci-coupling order n.

(iii) The structure of the logarithmic divergence (483), on the other hand, exhibits an "upward cascade" in orders of the Ricci-coupling. Namely, the ${}^0u_{2j}$ couplings will affect ${}^1Z_{2j}$, and more generally the renormalization constants ${}^nZ_{2j}$ associated to ${}^nU(\phi)R^n$ will be affected by all renormalized couplings of lower Ricci-coupling order ${}^0u_{2\ell}\,,\ldots,\,{}^nu_{2\ell}$.

(iv) This upward cascade in order of the Ricci-coupling halts within the "conformal sector", i.e.

$${}^1U(\phi) = \frac{1}{12}\phi^2\,,\quad {}^nU(\phi) \equiv 0\,,\quad n\geq 2\,, \tag{485}$$

but with general even scalar potential ${}^0U(\phi)$.

(v) In the standard case of a ϕ^4-theory, one may set ${}^nu_j = 0$ for all $n \geq 1$, $j \geq 0$ except for $\xi = {}^1u_2$, which corresponds to non-minimal coupling $\frac{1}{2}\xi\phi^2 R$ [81].

(vi) For a generic scalar potential ${}^0U(\phi)$ and non-conformal coupling ${}^1u_2 \neq 1/6$, the need to include Ricci-couplings of all orders in the action (441) follows from the structure of the logarithmic divergence, as can be readily seen by the following simple argument. Consider a sextic potential ${}^0U(\phi) = \frac{1}{2}m^2\phi^2 + \frac{1}{4!}\lambda\phi^4 + \frac{1}{6!}g\phi^6$ for non-conformal coupling. Then the logarithmic divergence in (472) contains the term

$$\frac{\hbar}{(4\pi)^2}\frac{1}{4!}\ln(\Lambda/\mu)({}^1u_2 - 1/6)g\phi^4 R\,, \tag{486}$$

to absorb which requires ${}^1u_4 \neq 0$ in the action (474). This in turn leads to the logarithmic divergence

$$\frac{\hbar}{(4\pi)^2}\frac{1}{2}\ln(\Lambda/\mu)({}^1u_2 - 1/6)\,{}^1u_4\phi^2 R^2\,, \tag{487}$$

which necessitates ${}^2u_2 \neq 0$, and so on.

(vii) In an attempt to avoid the infinite tower of Ricci couplings, one might try to remove some of the R^n divergences in (472) by a non-linear field renormalization

$$\begin{aligned}\phi_\Lambda &= \phi + \frac{\hbar}{(4\pi)^2}\ln(\Lambda/\mu)\,\zeta(\phi)R + O(\hbar^2)\,,\\ \zeta(\phi(\eta)) &= \sum_{n\geq 0}{}^n\zeta(\phi(\eta))R^n\,.\end{aligned} \tag{488}$$

In fact, since the upward cascade is triggered by the R^2 term in (487), removing this term would go a long way. However, since

$$S_\Lambda[\phi_\Lambda] = S_\Lambda[\phi] + \frac{\hbar}{(4\pi)^2}\ln(\Lambda/\mu)\int d\eta d^3x\, a^4\,\frac{\delta S}{\delta\phi}[\phi]\zeta(\phi) + O(\hbar^2)\,, \tag{489}$$

such a field renormalization does not produce any counterterms for on-shell background fields with $\delta S_\Lambda/\delta\phi = 0$. When keeping the background off-shell, a non-trivial $\zeta(\phi)$ clashes with a standard kinetic term and would require further modifications.

(viii) The tower

$$\sum_{n\geq 0}\sum_{j\geq 0}\frac{1}{(2j)!}\ {}^{n}u_{2j}\phi^{2j}R^{n} \tag{490}$$

is best organized by mass dimension. As noted after (442), the couplings

$${}^{n}u_{2j}\,,\quad n+j=N\,,\quad n\,,\,j\geq 0 \tag{491}$$

have mass dimension $4-2N$, and all but the $N=0,1,2$ ones are expected to become quickly subleading at large renormalization scale. In the following we compute the beta functions of these $1+2+3$ power counting non-irrelevant (i.e. power counting relevant and marginal) couplings,

$${}^{0}u_{0} \;=\; \frac{\Lambda_{\rm cosm}}{\kappa}\,,\qquad {}^{0}u_{2}=m^{2}\,,\qquad {}^{0}u_{4}=\lambda\,, \tag{492}$$

$${}^{1}u_{0} \;=\; -\frac{1}{\kappa}\,,\qquad {}^{1}u_{2}=\xi\,, \tag{493}$$

$${}^{2}u_{0} \;=\; \omega_{0}\,. \tag{494}$$

As usual we proceed by computing the renormalization constants ${}^{n}Z_{2j}$ by matching powers of $\phi^{2j}R^{n}$ between (477) and (479), (480). From the F_2-relation for the quadratic divergence (479) we obtain

$$\begin{aligned}
{}^{0}z_{2j,2}\ {}^{0}u_{2j} \;&=\; \mu^{2}q_{1,2}\ {}^{0}\bar{u}_{2j+2}\,,\quad j\geq 0\,,\\
{}^{1}z_{0,2}\ {}^{1}u_{0} \;&=\; \mu^{2}(q_{1,1}+q_{1,2}\ {}^{1}\bar{u}_{2})\,,\\
{}^{1}z_{2j,2}\ {}^{1}u_{2j} \;&=\; \mu^{2}q_{1,2}\ {}^{1}\bar{u}_{2j+2}\,,\quad j\geq 1\,,\\
{}^{n}z_{2j,2}\ {}^{n}u_{2j} \;&=\; \mu^{2}q_{1,2}\ {}^{n}\bar{u}_{2j+2}\,,\quad n\geq 2\,,j\geq 0\,,
\end{aligned} \tag{495}$$

while the logarithmic divergence (480) yields

$${}^{n}z_{2j,1}\ {}^{n}u_{2j} \;=\; \frac{1}{2}\sum_{\substack{n_1+n_2=n\\ n_1,n_2\geq 0}}\ \sum_{\substack{j_1+j_2=j\\ j_1,j_2\geq 0}}\frac{(2j)!}{(2j_1)!(2j_2)!}\ {}^{n_1}\bar{u}_{2j_1+2}\ {}^{n_2}\bar{u}_{2j_2+2}\,. \tag{496}$$

Beginning with the pure scalar sector, the renormalization constants for the power counting

non-irrelevant couplings (492) are

$$
\begin{aligned}
{}^0Z_0 &= 1+\frac{\hbar}{(4\pi)^2\ {}^0u_0}\Big\{\frac{1}{2}\ {}^0u_2^2\ln(\Lambda/\mu)+q_{1,2}\ {}^0u_2(\Lambda^2-\mu^2)+q_0(\Lambda^4-\mu^4)\Big\}\,,\\
{}^0Z_2 &= 1+\frac{\hbar}{(4\pi)^2\ {}^0u_2}\Big\{{}^0u_2\ {}^0u_4\ln(\Lambda/\mu)+q_{1,2}\ {}^0u_4(\Lambda^2-\mu^2)\Big\}\,,\\
{}^0Z_4 &= 1+\frac{\hbar}{(4\pi)^2\ {}^0u_4}\Big\{\big({}^0u_2\ {}^0u_6+3\ {}^0u_4^2\big)\ln(\Lambda/\mu)+q_{1,2}\ {}^0u_6(\Lambda^2-\mu^2)\Big\}\,,
\end{aligned}
\tag{497}
$$

while those of the higher couplings are

$$
\begin{aligned}
{}^0Z_{2j} &= 1+\frac{\hbar}{(4\pi)^2\ {}^0u_{2j}}\Big\{\frac{1}{2}\sum_{\substack{j_1+j_2=j\\ j_1,j_2\geq 0}}\left(\frac{(2j)!}{(2j_1)!(2j_2)!}\ {}^0u_{2j_1+2}\ {}^0u_{2j_2+2}\right)\ln(\Lambda/\mu)\\
&\quad+\ q_{1,2}\ {}^0u_{2j+2}(\Lambda^2-\mu^2)\Big\}\,,\quad j\geq 3\,.
\end{aligned}
\tag{498}
$$

Next, we present the renormalization constants for (493), (494)

$$
{}^1Z_0 = 1+\frac{\hbar}{(4\pi)^2\ {}^1u_0}\Big\{{}^0u_2\big({}^1u_2-\tfrac{1}{6}\big)\ln(\Lambda/\mu)+\big[q_{1,1}+q_{1,2}\big({}^1u_2-\tfrac{1}{6}\big)\big](\Lambda^2-\mu^2)\Big\}\,, \tag{499}
$$

$$
{}^1Z_2 = 1+\frac{\hbar}{(4\pi)^2\ {}^1u_2}\Big\{\big[\big({}^1u_2-\tfrac{1}{6}\big)\ {}^0u_4+{}^0u_2\ {}^1u_4\big]\ln(\Lambda/\mu)+q_{1,2}\ {}^1u_4(\Lambda^2-\mu^2)\Big\}\,, \tag{500}
$$

$$
{}^2Z_0 = 1+\frac{\hbar}{(4\pi)^2\ {}^2u_0}\Big\{\Big[\frac{1}{2}\big({}^1u_2-\tfrac{1}{6}\big)^2+{}^0u_2\ {}^2u_2\Big]\ln(\Lambda/\mu)+q_{1,2}\ {}^2u_2(\Lambda^2-\mu^2)\Big\}\,. \tag{501}
$$

Of course, $O(\hbar^2)$ corrections are implicit in all relations.

The flow equations for the couplings are derived by differentiating the defining relations: bare coupling = (renormalization constant) $\times$ (renormalized coupling) with respect to the scale μ. For the original (usually dimensionful) couplings, the response is always $O(\hbar)$ so that only the explicit μ-dependence needs to be taken into account. In a second step we then transition to dimensionless counterparts of the dimensionful couplings and rewrite the flow equations in terms of them. In preparation, we recall that the couplings ${}^nu_{2j}$ have mass dimension $4-2(n+j)$, and we denote their dimensionless counterparts by

$$
{}^nv_{2j} := \mu^{-4+2(n+j)}\ {}^nu_{2j}\,. \tag{502}
$$

The flow equations for the dimensionful pure scalar couplings are

$$\begin{aligned}
\mu\frac{d}{d\mu}{}^0u_0 &= \frac{\hbar}{(4\pi)^2}\Big\{4q_0\mu^4 + 2q_{1,2}\,{}^0u_2\mu^2 + \frac{1}{2}\,{}^0u_2^2\Big\}\,, \qquad (503)\\
\mu\frac{d}{d\mu}{}^0u_2 &= \frac{\hbar}{(4\pi)^2}\Big\{2q_{1,2}\,{}^0u_4\mu^2 + {}^0u_2\,{}^0u_4\Big\}\,,\\
\mu\frac{d}{d\mu}{}^0u_4 &= \frac{\hbar}{(4\pi)^2}\Big\{2q_{1,2}\,{}^0u_6\mu^2 + 3\,{}^0u_4^2 + {}^0u_2\,{}^0u_6\Big\}\,,\\
\mu\frac{d}{d\mu}{}^0u_{2j} &= \frac{\hbar}{(4\pi)^2}\Big\{2q_{1,2}\,{}^0u_{2j+2}\mu^2 + \frac{1}{2}\sum_{\substack{j_1+j_2=j\\ j_1,j_2\geq 0}}\frac{(2j)!}{(2j_1)!(2j_2)!}\,{}^0u_{2j_1+2}\,{}^0u_{2j_2+2}\Big\}\,,\quad j\geq 3\,,
\end{aligned}$$

while those of their dimensionless counterparts read

$$\begin{aligned}
\mu\frac{d}{d\mu}\varepsilon &= -4\varepsilon + \frac{\hbar}{(4\pi)^2}\Big\{4q_0 + 2q_{1,2}\,{}^0v_2 + \frac{1}{2}\,{}^0v_2^2\Big\}\,, \qquad (504)\\
\mu\frac{d}{d\mu}{}^0v_2 &= -2\,{}^0v_2 + \frac{\hbar}{(4\pi)^2}\Big\{2q_{1,2}\,{}^0v_4 + {}^0v_2\,{}^0v_4\Big\}\,,\\
\mu\frac{d}{d\mu}{}^0v_4 &= \frac{\hbar}{(4\pi)^2}\Big\{2q_{1,2}\,{}^0v_6 + 3\,{}^0v_4^2 + {}^0v_2\,{}^0v_6\Big\}\,,\\
\mu\frac{d}{d\mu}{}^0v_{2j} &= (2j-4)\,{}^0v_{2j}\\
&\quad + \frac{\hbar}{(4\pi)^2}\Big\{2q_{1,2}\,{}^0v_{2j+2} + \frac{1}{2}\sum_{\substack{j_1+j_2=j\\ j_1,j_2\geq 0}}\frac{(2j)!}{(2j_1)!(2j_2)!}\,{}^0v_{2j_1+2}\,{}^0v_{2j_2+2}\Big\}\,,\quad j\geq 3\,,
\end{aligned}$$

where we denote the dimensionless vacuum energy by $\varepsilon := {}^0v_0 = \mu^{-4}\,{}^0u_0$. These equations are precisely those obtained on a flat spacetime, and are not closed as the one for ${}^0v_{2j}$ also invokes ${}^0v_{2j+2}$, $j\geq 0$. In order to solve them a truncation is required that sets all ${}^0v_{2j}$ to zero for all $j\geq j_0$, for some $j_0\in\mathbb{N}$. Truncation at order $j_0 = 4$ yields the fixed point

$$\varepsilon^* = \frac{\hbar}{(4\pi)^2}q_0\,,\quad {}^0v_2^* = {}^0v_4^* = {}^0v_3^* = 0\,, \qquad (505)$$

consistent with the existence of only a Gaussian fixed point for a scalar theory in four spacetime dimensions. It is noteworthy, however, that the dimensionless vacuum energy ε has a mass independent positive fixed point that depends only mildly on the choice of the regulator. This is also a feature of the local potential approximation (LPA) truncation of the FRG, but it cannot be seen in dimensional regularization.

Next, we proceed to the power counting non-irrelevant higher order (dimensionful) Ricci couplings (493), (494), whose running is determined by (499)-(501)

$$\begin{aligned}
\mu\frac{d}{d\mu}{}^1u_0 &= \frac{\hbar}{(4\pi)^2}\Big\{\big({}^0u_2+2q_{1,2}\mu^2\big)\big({}^1u_2-1/6\big)+2q_{1,1}\mu^2\Big\},\\
\mu\frac{d}{d\mu}{}^1u_2 &= \frac{\hbar}{(4\pi)^2}\Big\{\big({}^1u_2-1/6\big)\ {}^0u_4+{}^0u_2\ {}^1u_4+2q_{1,2}\ {}^1u_4\mu^2\Big\},\\
\mu\frac{d}{d\mu}{}^2u_0 &= \frac{\hbar}{(4\pi)^2}\Big\{\frac{1}{2}\big({}^1u_2-1/6\big)^2+{}^0u_2\ {}^2u_2+2q_{1,2}\ {}^2u_2\mu^2\Big\}.
\end{aligned}\tag{506}$$

The first equation transcribes into a flow equation for the dimensionless Newton constant $\mathrm{g}_N=\mu^2\kappa$ via ${}^1v_0=-1/(2\mathrm{g}_N)$,

$$\mu\frac{d}{d\mu}\mathrm{g}_N = 2\mathrm{g}_N+\frac{\hbar}{(4\pi)^2}\Big\{4q_{1,1}\mathrm{g}_N^2+\big({}^0v_2+2q_{1,2}\big)\big({}^1v_2-1/6\big)\mathrm{g}_N^2\Big\},\tag{507}$$

while the remaining two yield

$$\begin{aligned}
\mu\frac{d}{d\mu}{}^1v_2 &= \frac{\hbar}{(4\pi)^2}\Big\{\big({}^1v_2-1/6\big)\ {}^0v_4+{}^0v_2\ {}^1v_4+2q_{1,2}\ {}^1v_4\Big\},\\
\mu\frac{d}{d\mu}{}^2v_0 &= \frac{\hbar}{(4\pi)^2}\Big\{\frac{1}{2}\big({}^1v_2-1/6\big)^2+{}^0v_2\ {}^2v_2+2q_{1,2}\ {}^2v_2\Big\}.
\end{aligned}\tag{508}$$

The flow equation (507) admits a nontrivial fixed point that is best interpreted as the one for the $1/\mathrm{g}_N$ flow,

$$1/\mathrm{g}_N^* = -\frac{\hbar}{2(4\pi)^2}\Big\{4q_{1,1}+\big({}^0v_2^*+2q_{1,2}\big)\big({}^1v_2-1/6\big)\Big\},\tag{509}$$

where typically ${}^0v_2^*=0$ by (505). We note that compared to the covariant formulation, the beta function (507) and fixed point (509) feature an additional contribution proportional to $q_{1,1}$ arising from the time dependence of the spatial regulator (446). Since $q_{1,1}>0$ this contribution (as is typical of matter) tends to drive the Newton coupling to negative values. However, in a full quantum gravity plus matter computation one expects that the quantum gravity will turn g_N^* positive again. Furthermore, it is noteworthy that this additional contribution from the spatial averaging does not vanish for conformal coupling to matter.

6.3 Conclusions

In this chapter, we have presented the FLFRG or spatial FRG, which is a novel manifestly Lorentzian formulation of the (normally Euclidean) Functional Renormalization Group technique. The transition from Euclidean to Lorentzian signature necessitates the use of a merely spatial mode modulator, which has not been studied for generic Friedmann-Lemaître spacetimes. UV boundary data for the flow equation has been prepared through a one-loop computation, with these boundary data injecting the form of the bare action. Instead of the usual regularized trace-log computation, one can use the spatial FRG itself to extract the divergent parts of the one-loop effective action. In this way, consistency with the subsequent use of the one-loop computation as setting boundary data is built in. This was accomplished utilizing generalized resolvent expansion from Chapter 5, thereby the avoiding the ill-defined pseudo-heat kernel techniques. These UV divergent parts were subsequently cancelled by counterterms in the bare action, as usual. Among the infinitely many Wilsonian couplings, only six are power counting non-irrelevant, and their renormalization flow has been presented. We further highlight several noteworthy features:

(i) Surprisingly, although the spatial regulator breaks spacetime covariance, only *covariant* counterterms are needed to renormalize the effective action associated to the bare action (441) to one-loop order.

(ii) One-loop renormalization of a pure scalar potential beyond quartic order generically necessitates an infinite tower of Ricci couplings in the bare action (441). The only exception is the strictly conformal coupling of gravity to matter, wherein a general scalar potential can be renormalized.

(iii) The renormalization structure entailed by (476), (482), (483) exhibits an "upward cascading" in the Ricci-coupling order n, i.e. the couplings ${}^0u_{2j}, \ldots, {}^nu_{2j}$ determine the running of ${}^nu_{2j}$.

(iv) The time dependence of the spatial regulator kernel R_k through the cosmological scale factor (446) induces an additional quadratic divergence that affects the running of the Newton constant. In particular, the Newton constant runs even for conformally

coupled gravity and matter fields. In a full quantum gravity computation, this would quantitatively affect the interplay between the matter and gravity sectors.

(v) In the context of the FLFRG proper, the one-loop renormalization flow studied would set the boundary conditions for the spatial LPA (39). The numerical evolution of the coupling flow will draw on the overall framework developed in earlier chapters, in particular analytical control of the field dependence in the Green function. It is here where the specifics of the state enters, which will affect the small k behavior of the flow.

7.0 Conclusions

The current cosmological paradigm posits the validity of general relativity almost up to the Big Bang. This entails that the Einstein equations can be used to study the detailed structure of spacetime in the vicinity of the (spacelike) singularity. A major qualitative feature of these studies is that spatial gradients become subleading compared to temporal ones. Combined with the presumed gravitational simplicity of the Big Bang singularity, one is led to model it as a quiescent (i.e. non-oscillatory) singularity. This ties into the narrower cosmological paradigm wherein the classical spacetime is thought to be well approximated by a (spatially flat) Friedmann-Lemaître spacetime driven by a homogeneous scalar field, and a description of physics in terms of quantum field theories on such a curved background is deemed to be valid. Within this narrower framework, the focus is normally on the exponentially expanding deSitter-like period. However, it must be stressed that within the same premises a non-accelerated pre-inflationary period is mandated by general relativity [38, 2].

Accepting this physically well-motivated scenario of the existence of a pre-inflationary phase, during which the description of QFT on curved backgrounds is expected to be valid, the aim of this thesis has been to develop a customized theoretical framework for interacting scalar QFTs on generic Friedmann-Lemaître backgrounds. Such a framework cannot be in Euclidean signature as the expanding spacetime generically prohibits a Wick rotation [6], nor should it be tailored towards de Sitter spacetime. Motivated by the subdominance of spatial gradients, we aimed at developing variants of a spatial gradient expansion in the very early Universe. Moreover, since the classical potential underlying the inflationary paradigm is typically non-renormalizable, we wish to de-emphasize weak coupling and the specific form of the potential in the formalism. In renormalization group language, this suggests a Wilsonian approach, where all interaction monomials compatible with some prescribed symmetry are initially treated on the same footing. However, the standard approaches which are Wilsonian in spirit, namely lattice methods or the Functional Renormalization Group, strongly rely on Euclidean signature. In the present context, this necessitates a new adaptation of Wilsonian ideas to Friedmann-Lemaître spacetimes.

In Chapter 2 we presented the Anti-Newtonian expansion in a spatially discretized setting, where the flat spatial sections of the Friedmann-Lemaître background are replaced with a hypercubical lattice $(a_s\mathbb{Z})^d$ of spacing a_s. This discretized expansion can be recast as a spatial hopping (linked cluster) expansion, which allowed us to partially adapt existing methodology. In this framework, the solution of the QFT decouples into two sub-problems: (1) the solution of the cosmological quantum mechanics, conceptually associated with the decoupled wordlines in the Anti-Newtonian limit; and (2) the solution of the combinatorial problem that allows one to analytically control the terms of the linked cluster expansion, which is conceptually associated with restoring the spatial interaction between the neighboring world lines. With the goal of making contact to the Functional Renormalization Group, we focused in Chapter 3 on developing a linked cluster expansion for the Legendre effective action. The resulting graph rules are largely model independent (unlike Feynman rules). Moreover, the covariant Euclidean results from Chapter 3 can easily be adapted to the spatially discretized setting on a generic Friedmann-Lemaître background, see Section 2.2.

In Chapter 4 we have presented a "proof-of-principle" study showing that the Functional Renormalization Group can be applied to efficiently calculate the critical parameters of the hopping expansion of Euclidean ϕ_3^4, ϕ_4^4 theory. Motivated by this, as well as the role of the FRG in the asymptotic safety scenario, we proceeded to develop the elements needed for a manifestly Lorentzian formulation of the FRG. One of the key differences of this formulation compared to the Euclidean setting is that it necessitates the incorporation of state-dependent data directly into the flow equation formalism. Specifically, in the local potential approximation (LPA) to the FRG, the right hand side of the flow equation is governed by a Green function of a mode modulated free wave operator. As a consequence, choices analogous to the selection of a state for perturbative QFTs on curved backgrounds need to be made (see Figure 2). One is thus led to construct Green functions on a Friedmann-Lemaître background with the Hadamard property. The Hadamard property entails a universal UV behavior of the resulting LPA flow, while the infrared properties will inevitably be state-dependent.

In Chapter 5 we therefore studied a well-motivated class of vacuum states defined on generic Friedmann-Lemaître backgrounds, so-called States of Low Energy (SLE). In addition

to being Hadamard states, we prove that they have a number of additional properties that make them even more appealing. In particular, they allow for a controlled infrared expansion on *generic* Friedmann-Lemaître backgrounds. In the context of the FRG, this mathematically defines the LPA at all scales, in sharp contrast to the commonly used (pseudo-) heat kernel methodology, which inevitably reorganizes only ultraviolet information. One application is a novel resolution of the infrared divergences that plague massless modes on many Friedmann-Lemaître backgrounds. In this setting, SLE have the remarkable property of a universal Minkowski-like *infrared* behavior, yielding infrared finite two-point functions. This feature impacts the primordial power spectrum, computed for modes based on a SLE, modifying the low angular momentum parts in a way compatible with current CMB data. We close this chapter by presenting a simple generalization of the SLE construction to a one-parameter family of Hadamard states, which we envision as being fruitful for the LPA.

Finally, in Chapter 6 we presented the spatial FRG and prepared UV boundary data for it. These boundary data inject the Wilsonian one-loop flow associated to the bare action. Instead of the usual regularized trace-log computation, one can use the spatial FRG itself to extract the divergent parts of the one-loop effective action. In this way, consistency with the subsequent use of the one-loop computation as setting boundary data is built in. Technically, this was done by utilizing generalized resolvent expansion from Chapter 5, thereby avoiding the ill-defined pseudo-heat kernel techniques. Despite the non-covariant spatial regulator, the UV divergent parts come out as spacetime covariant (although slightly different from the formal use of a covariant regulator). These UV divergent parts were subsequently cancelled by counterterms in the bare action, as usual. Among the infinitely many Wilsonian couplings, only six are power counting non-irrelevant, and their renormalization flow has been presented. Of particular note is the additional contribution to the renormalization of the Newton constant, induced by the time dependence of the regulator through the cosmological scale factor. In a full quantum gravity computation, this would quantitatively affect the interplay between the matter and gravity sectors. Within the context of the asymptotic safety scenario, it is believed that the interplay between the gravity and matter couplings resolves the triviality of scalar field theories. This has found phenomenological applications, which are however as yet provisionary, because the infrared regime of the flow equation is

neither well-posed or controlled. This thesis prepares the tools to address this situation.

Appendix A Graph Rules for the Linked Cluster Expansion of the Legendre Effective Action

A.1 Recursive results to fifth order

Here we present explicit results for Γ_l, $l = 2, \dots, 5$, and various checks on them. A closed recursion arises from the expansion of the κ-flow equation in (79). In preparation we define polynomials $m_l = m_l(u_1, \dots, u_l)$ in non-commuting variables u_n, $n \in \mathbb{N}$, by

$$\left(1+\sum_{n\geq 1}\kappa^n u_n\right)\left(1-\sum_{l\geq 1} m_l(u)\kappa^l\right) = 1 = \left(1-\sum_{l\geq 1} m_l(u)\kappa^l\right)\left(1+\sum_{n\geq 1}\kappa^n u_n\right),$$
$$m_l(u) = \sum_{n=1}^{l}\sum_{i_1+\dots+i_n=l, i_j\in\mathbb{N}} (-)^{n+1}\, u_{i_1}\dots u_{i_n}\,. \tag{510}$$

At low orders: $m_1 = u_1$, $m_2 = u_2 - u_1^2$, $m_3 = u_3 - u_1u_2 - u_2u_1 + u_1^3$. Inserted into (79) one has $\Gamma_1 \equiv 0$ and

$$\Gamma_l = \frac{1}{2l}\sum_{n=1}^{l-1}\sum_{i_1+\dots+i_n=l-1} (-)^n \,\mathrm{Tr}[u_1 u_{i_1}\dots u_{i_n}]\,, \quad l \geq 2\,, \tag{511}$$

with $\Gamma_0^{(2)}\cdot u_1 = \ell$, $\Gamma_0^{(2)}\cdot u_i = \Gamma_i^{(2)}$, $i \geq 2$. Here $\Gamma_0^{(2)}[\phi]$ is invertible

$$\Gamma_0^{(2)}[\phi]_{x,y} = \gamma_2(\phi_x)\delta_{x,y}\,, \quad \gamma_2(\varphi)^{-1} = \omega_2|_{h=h(\varphi)}\,. \tag{512}$$

In slight abuse of notation we set $\omega_i(\varphi) := \omega_i(h(\varphi))$, $\omega_i(h) = \partial^i\omega/\partial h^i$, $i \geq 2$, and find:

$$\begin{aligned}
\Gamma_2[\phi] &= -\sum_{x_1,x_2}\frac{1}{4}\omega_2(\phi_{x_1})\omega_2(\phi_{x_2})(\ell_{x_1x_2})^2 \\
\Gamma_3[\phi] &= \sum_{x_1,x_2}\frac{1}{12}\omega_3(\phi_{x_1})\,\omega_3(\phi_{x_2})\,(\ell_{x_1x_2})^3 \\
&+ \sum_{x_1,x_2,x_3}\frac{1}{6}\omega_2(\phi_{x_1})\omega_2(\phi_{x_2})\omega_2(\phi_{x_3})\ell_{x_1x_2}\,\ell_{x_2x_3}\,\ell_{x_1x_3} \\
\Gamma_4[\phi] &= -\sum_{x_1,x_2}\frac{1}{48}\omega_4(\phi_{x_1})\omega_4(\phi_{x_2})(\ell_{x_1x_2})^4
\end{aligned} \tag{513}$$

$$
\begin{aligned}
&- \sum_{x_1,x_2,x_3} \frac{1}{4}\omega_3(\phi_{x_1})\,\omega_3(\phi_{x_2})\,\omega_2(\phi_{x_3})(\ell_{x_1x_2})^2\,\ell_{x_1x_3}\,\ell_{x_2x_3} \\
&- \sum_{x_1,x_2,x_3} \frac{1}{8}\omega_2(\phi_{x_1})\,[\omega_4-\omega_3\gamma_2\omega_3](\phi_{x_2})\,\omega_2(\phi_{x_3})(\ell_{x_1x_2})^2\,(\ell_{x_2x_3})^2 \\
&- \sum_{x_1,x_2,x_3,x_4} \frac{1}{8}\omega_2(\phi_{x_1})\omega_2(\phi_{x_2})\omega_2(\phi_{x_3})\omega_2(\phi_{x_4})\ell_{x_1x_2}\,\ell_{x_2x_3}\,\ell_{x_3x_4}\,\ell_{x_4x_1}\,.
\end{aligned}
$$

$$
\begin{aligned}
\Gamma_5[\phi] &= \sum_{x_1,x_2} \frac{1}{120}\omega_5(\phi_{x_1})\omega_5(\phi_{x_2})(\ell_{x_1x_2})^5 \\
&+ \sum_{x_1,x_2,x_3} \frac{1}{12}\omega_4(\phi_{x_1})\omega_4(\phi_{x_2})\omega_2(\phi_{x_3})(\ell_{x_1x_2})^3\ell_{x_1x_3}\ell_{x_2x_3} \\
&+ \sum_{x_1,x_2,x_3} \frac{1}{12}\omega_2(\phi_{x_1})\big[\omega_5-\omega_3\gamma_2\omega_4\big](\phi_{x_2})\omega_3(\phi_{x_3})(\ell_{x_1x_2})^2(\ell_{x_2x_3})^3 \\
&+ \sum_{x_1,x_2,x_3} \frac{1}{8}\omega_3(\phi_{x_1})\omega_3(\phi_{x_2})\omega_4(\phi_{x_3})\ell_{x_1x_2}(\ell_{x_1x_3})^2(\ell_{x_2x_3})^2 \qquad (514) \\
&+ \sum_{x_1,x_2,x_3,x_4} \frac{1}{4}\omega_2(\phi_{x_1})\omega_2(\phi_{x_2})\omega_3(\phi_{x_3})\omega_3(\phi_{x_4})\ell_{x_1x_2}\ell_{x_2x_3}(\ell_{x_3x_4})^2\ell_{x_4x_1} \\
&+ \sum_{x_1,x_2,x_3,x_4} \frac{1}{4}\omega_3(\phi_{x_1})\omega_2(\phi_{x_2})\omega_3(\phi_{x_3})\omega_2(\phi_{x_4})\ell_{x_1x_2}\ell_{x_2x_3}\ell_{x_3x_4}\ell_{x_4x_1}\ell_{x_1x_3} \\
&+ \sum_{x_1,x_2,x_3,x_4} \frac{1}{4}\omega_2(\phi_{x_1})\omega_2(\phi_{x_2})\big[\omega_4-\omega_3\gamma_2\omega_3\big](\phi_{x_3})\omega_2(\phi_{x_4})\ell_{x_1x_2}\ell_{x_2x_3}\ell_{x_3x_1}(\ell_{x_3x_4})^2 \\
&+ \sum_{x_1,x_2,x_3,x_4,x_5} \frac{1}{10}\omega_2(\phi_{x_1})\omega_2(\phi_{x_2})\omega_2(\phi_{x_3})\omega_2(\phi_{x_4})\omega_2(\phi_{x_5})\ell_{x_1x_2}\ell_{x_2x_3}\ell_{x_3x_4}\ell_{x_4x_5}\ell_{x_5x_1}\,.
\end{aligned}
$$

A computational point worth mentioning is that the $(\Gamma_m^{(2)})_{xy}$, $m \geq 2$, have in general diagonal elements. In evaluating the traces one has to split off at intermediate steps subsums containing $(\Gamma_m^{(2)})_{xx}$ contributions. Such contributions combine with others and lead to unrestricted sums in the final result, but with modified coefficients.

The corresponding W_l's are readily obtained from the Wortis graph rule and are not displayed explicitly. In line with table 1 the expressions for the Γ_l are (at matching orders) more concise than the W_l's and yet code the same information. These results have been tested and compared with partial results in the literature in various ways. (i) $W_1, \ldots, W_4$ and $\Gamma_2, \ldots, \Gamma_5$ are related by the mixed recursion (90). (ii) Specialized to the Ising model

$\Gamma_2, \ldots, \Gamma_4$ agree with the resuls of [97].

The $W_1, \ldots, W_4$ themselves can be specialized to a nearest neighbor hopping matrix and matched to results in the literature. (iii) For $H = 0$ the textbook result for the free energy is reproduced. (iv) The 2-point susceptibility $\chi_2 = \sum_x W^{(2)}_{x,0}|_{H=0}$ and the 4-point susceptibility $\chi_4 = \sum_{x_1,x_2,x_3} W^{(4)}_{x_1,x_2,x_3,0}|_{H=0}$ match (in $d = 2$) the results in [5].

A.2 Single site data and zero-dimensional Legendre transform

The function $\gamma(\varphi)$ entering the ultralocal initial functional $\Gamma_0[\phi] = \sum_x \gamma(\phi_x)$ can be characterized by the functional relation

$$\exp\Big(-\gamma(\varphi)\Big) = \int_{-\infty}^{\infty} d\chi \, \exp\Big\{-s(\chi) + (\chi - \varphi)\frac{\partial \gamma}{\partial \varphi}\Big\}, \tag{515}$$

where s is the single site action. By shifting the argument $\varphi \mapsto \varphi + \alpha$ and expanding in powers if α one can express the derivatives $\gamma_n(\varphi) = \partial^n \gamma / \partial \varphi^n$ in terms of the cumulants $\omega_n(h) = \partial^n \omega / \partial h^n$ of the measure $d\chi e^{-s(\chi)}$. The latter have generating function $e^{\omega(h+k)} = \int d\chi \exp\{-s(\chi) + (h+k)\chi\}$ upon expansion in powers of k. To low orders one finds

$$\gamma_2(\varphi) = \omega_2^{-1}|_{h=h(\varphi)}\,, \quad \gamma_3(\varphi) = -\omega_2^{-3}\omega_3|_{h=h(\varphi)}\,, \quad \gamma_4(\varphi) = [-\omega_4\omega_2^{-4} + 3\omega_3^2\omega_2^{-5}]_{h=h(\varphi)}\,. \tag{516}$$

Augmented by $\omega_1|_{h=h(\varphi)} = \varphi$ and $\gamma_1(\varphi) = h(\varphi)$ the inverse relations are obtained by flipping the roles of the ω_m's and γ_m's. This reflects the fact that the generating functions $\omega(h+k)$ and $\gamma(\varphi+\alpha)$ are Legendre transforms of each other. In quantum field theoretical terminology the $\gamma_l(\varphi)$ are zero-dimensional vertex functions with non-zero mean field and the $\omega_l(h)$ are the zero-dimensional cumulants with non-zero source.

The combinatorial patterns arising through the Legendre transform can be analyzed in closed form in the zero dimensional case. The integral realization does not enter, so $\omega : \mathbb{R} \to \mathbb{R}$, can be any smooth function with nonzero second derivative, $\omega^{(2)}(h) > 0$, say. We assume that $\omega^{(1)}(h) = \varphi$ can be solved for $h(\varphi)$, where h is likewise smooth and $h^{(1)}(\varphi) > 0$. We define the Legendre transform by $\gamma(\varphi) := \varphi h(\varphi) - \omega(h(\varphi))$. Then $\gamma^{(1)}(\varphi) = h(\varphi)$ and

the primary assertion is that $\omega^{(1)}$ and $\gamma^{(1)}$ are compositional inverses of each other

$$\omega^{(1)}(\gamma^{(1)}(\varphi)) = \varphi\,, \quad \gamma^{(1)}(\omega^{(1)}(h)) = h\,. \tag{517}$$

By repeated differentiation of these basic formulas one can generate relations between the derivatives $\gamma_l(\varphi) := \gamma^{(l)}(\varphi)$ and the $\omega_l(h) := \omega^{(l)}(h)$. For now we focus on $\omega^{(1)}(\gamma^{(1)}(\varphi)) = \varphi$, where the first few relations generated are (516). Since the resulting $\omega(h)$ derivatives are always evaluated at $h = h(\varphi) = \gamma^{(1)}(\varphi)$ it is convenient to set $\omega_m(\varphi) := \omega_m(h)|_{h=h(\varphi)}$ by slight abuse of notation. In this notation ∂_φ is a linear derivation acting via $\partial_\varphi \omega_n = \omega_{n+1}\gamma_2$ and $\partial_\varphi \gamma_n = \gamma_{n+1}$ on the constituents. The differentiation rule implies that the l-th order relation has the form

$$\omega_2^l \gamma_l = -\omega_l \; + \sum_{-2i_2+3i_3+\ldots+(l-1)i_{l-1}=l} (-)^{i_3+\ldots+i_{l-1}} c_{i_3\ldots i_{l-1}} \, (\omega_2^{-1})^{i_2} \omega_3^{i_3} \ldots \omega_{l-1}^{i_{l-1}}\,, \quad l \geq 4\,, \tag{518}$$

for $i_k \in \mathbb{N}$ and integer coefficients $c_{i_3\ldots i_{l-1}} \in \mathbb{N}$. Unless noted otherwise the ω_m in the following are the $\omega_m(\varphi) = \omega_m(h)|_{h=h(\varphi)}$ regarded as functions of φ.

The coefficients $c_{i_3\ldots i_{l-1}}$ are indirectly characterized by the duality property (517): solving (518) recursively for the ω_l in terms of $\gamma_2, \ldots, \gamma_l$, the same formula arises. An explicit formula for them arises from the known combinatorial expressions for the compositional inverse:

$$c_{i_3\ldots i_{l-1}} = \Big(l-2+\textstyle\sum_{j=3}^{l-1} i_j\Big)! \displaystyle\prod_{j=3}^{l-1} \frac{1}{i_j!(j-1)!^{\,i_j}}\,. \tag{519}$$

This has been obtained in [53] in a setting that mimics perturbation theory; the functions are power series in the fields and the numerical coefficients are related as in (519). A little thought shows that the coefficients arising through repeated differentiation of arbitrary smooth functions without setting the argument to zero are the same. For later reference we sketch the argument.

The basic input is an explicit expression for the compositional inverse of a formal power series. There are several variants of such formulas and their tree-graph interpretation; the version most directly leading to (519) is Eq. (4.6) in [93]. Given $a(z) = \sum_{n\geq 1} a_n z^n$, $a_1 \neq 0$,

the series $b(w) = \sum_{n\geq 1} \frac{b_n}{n!}\, w^n$ is the compositional inverse of a, i.e. $a(b(w)) = w$, iff

$$b_n = \sum_{k_2,k_3,\ldots\geq 0, \sum_j (j-1)k_j = n-1} (-)^{\sum_j k_j}\, a_1^{-(1+\sum_j jk_j)} \Big(\sum_j jk_j\Big)! \prod_j \frac{a_j^{k_j}}{k_j!}\,, \tag{520}$$

where all sums and products range over $j \geq 2$ and are rendered finite by the Euler relation $\sum_j (j-1)k_j = n-1$. For the application here we shift the arguments of ω and γ and re-expand. For the first derivatives this gives

$$\begin{aligned} \omega^{(1)}(h+k) &= \sum_{n\geq 0} \frac{k^n}{n!} \omega_{n+1}(h) =: \omega^{(1)}(h;k)\,, \\ \gamma^{(1)}(\varphi+\alpha) &= \sum_{n\geq 0} \frac{\alpha^n}{n!} \gamma_{n+1}(\varphi) =: \gamma^{(1)}(\varphi;\alpha)\,. \end{aligned} \tag{521}$$

By (517) we require both series to be compositional inverses of each other as series in k, α. The result (519) then follows from (520).

The formula (520) has several known combinatorial and tree graph interpretations, see [33, 93, 53] and the references therein. In the remainder of this appendix we present a graph theoretical interpretation of (518), (519) which, together with its proof, mirrors some aspects of its quantum field theoretical counterpart in Section 3.3.

Graph rules for γ_l:

(i) At order $l \geq 4$ draw all topologically distinct connected tree graphs $t \in \mathcal{T}_l$ with $l = |\nu_0|$ external vertices of order 1 and any number $|\nu_1|$ of k-valent vertices, $k = 3, \ldots, l$, joined by dashed lines. Multiply by $l!/|\mathrm{Aut}(t)| \in \mathbb{N}$, where $\mathrm{Aut}(t)$ is the automorphism group of the graph.

(ii) Attribute to each $t \in \mathcal{T}_l$ a weight $(-)^{|\nu_1|}\mu(t)$ as follows: a factor ω_2^{-1} to each dashed line, 1 to an 1-valent vertex, and $-\omega_k$ to an k-valent vertex, $k \geq 3$.

(iii) Sum over all contributions to obtain

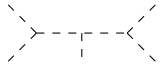
$$\gamma_l = \sum_{t\in\mathcal{T}_l} (-)^{|\nu_1|} \frac{l!}{|\mathrm{Aut}(t)|} \mu(t)\,, \quad \text{i.e.} \quad c_{i_3\ldots i_{l-1}} = l! \sum_{t\in\mathcal{T}_{i_3\ldots i_{l-1}}} \frac{1}{|\mathrm{Aut}(t)|}\,, \tag{522}$$

where the c's are those in (518) and the graphs contributing to a fixed $\mu(t)$ with labels $(i_3 \ldots i_{l-1})$ are denoted by $\mathcal{T}_{i_3\ldots i_{l-1}} \subset \mathcal{T}_l$.

The automorphism group in (i) is defined as in Section 3.2.1, with ν_0 the set of external vertices, ν_1 the set of multi-valent vertices, and edge list $\epsilon \subset (\nu_0 \cup \nu_1)_2$. The Euler relations holds in the form $|\nu_0| + |\nu_1| = |\epsilon| + 1$ and $\sum_{k=1}^{l} k|v|_k = 2|\epsilon|$, where $|v|_k$ is the number of k-valent vertices, $k = 1, 3, 4, \ldots$. The second form ensures that the degrees and signs in (518) are correctly reproduced by (ii) and only the coefficients $c_{i_3 \ldots i_{l-1}}$ in (iii) need to be understood in graph theoretical terms. Importantly, for $l \geq 6$ several topologically distinct tree graphs contributing to a fixed a $(i_3 \ldots i_{l-1})$ configuration can occur. As an example, the tree graphs contributing to γ_5 are displayed below

$$\omega_2^{-5}\omega_5 \qquad |\mathrm{Aut}(t)| = 5!$$

$$\omega_2^{-6}\omega_3\omega_4 \qquad |\mathrm{Aut}(t)| = 3!2!$$



$$\omega_2^{-7}\omega_3^3 \qquad |\mathrm{Aut}(t)| = 2^3 \tag{523}$$

A proof of (522) can be based on the known tree graph interpretation of (520), see [53, 93] and the references therein. Below we provide an alternative ab-initio proof without reference to the compositional inverse formula. The key ingredient is the following mixed recursion relation

$$\gamma_l(\varphi) = -\sum_{j=2}^{l} \omega_j(\varphi) \frac{l!}{j!} \sum_{k_1+\ldots+k_j=l,\, 1\leq k_i\leq l-2} \frac{\gamma_{k_1}^{(1)}(\varphi)}{k_1!} \cdots \frac{\gamma_{k_j}^{(1)}(\varphi)}{k_j!}\,, \quad l \geq 3\,. \tag{524}$$

This is the zero-dimensional counterpart of the recursions (90), (98) instrumental for our analysis of the Γ_κ graph rules. It can be derived along similar lines starting from $\gamma(\varphi+\alpha) = (\varphi+\alpha)\gamma^{(1)}(\varphi;\alpha) - \omega(\gamma^{(1)}(\varphi;\alpha))$ and (521).

Ab-initio proof of γ_l graph rule based on (524). We proceed by induction in l, assuming that (522) is known to produce the correct coefficients (522) for $k = 1, \ldots, l-1$. To obtain the result at order l we first note a simple generation recipe $(*)$: the set of tree graphs in $\mathcal{T}_{k-1}$ can be obtained from those in $\mathcal{T}_{k-2}$ by insertion of a line in all possible ways either at a multi-valent vertex or in the middle of an existing line. In fact, differentiating a weight

of order $k-2$ from part (ii) of the graph rule, $\partial_\varphi \mu(t)$, produces a sum of terms whose interpretation as order $k-1$ tree graphs follows the pattern $(*)$. The terms occur with integer multiplicities which by the origin of (518) from (517) must be compatible with (522).

The recursion (524) also mirrors the pattern $(*)$. Fix some $t \in \mathcal{T}_l$ generated from order $l-1$ graphs as indicated. The contribution of t to $\gamma_l/l!$ can be matched to terms on the right hand side of (524) in the following way. Case 1: any $3 \leq j$-valent internal vertex can be seen as the ω_j piece, and the j subtrees it connects to as the 1-rooted $\gamma^{(1)}_{k_i}/k_i!$ pieces. Case 2: the middle of an internal line with adjacent vertices of weights $\omega_{n_1}, \omega_{n_2}$ can be seen as an ω_2 pseudo-vertex via $\omega_{n_1}\omega_2^{-1}\omega_{n_2} = \partial_\varphi \omega_{n_1-1}\omega_2 \partial_\varphi \omega_{n_2-1}$, and the two subtrees it connects to as 1-rooted $\gamma^{(1)}_{k_i}/k_i!$ pieces. The full contribution of t obtained from (524) is then the sum of reassembled rooted graph weights produced by each distinct choice of the ω_j, $j \geq 2$, and $\gamma^{(1)}_{k_i}$ pieces. Our task is to keep track of the coefficients.

Case 1: j-valent vertex as ω_j, $j \geq 3$. By induction hypothesis each of the γ_{k_i} has a graph realization in $\mathcal{T}_{k_1}$ via (i),(ii),(iii). Its derivative $\gamma^{(1)}_{k_i}$ has the same structure where initially the differentiated weights $\partial_\varphi \mu(t)$ occur. By the remark following $(*)$ each $\partial_\varphi \mu(t)$ expands into tree graphs of one order higher which we regard as 1-rooted, $t' \in \mathcal{T}^{1\bullet}_{k_i+1}$ (with the rooted vertex always an internal one). The regrouping leads to coefficients of the $\mu(t')$'s that must by the differentiation compatibility be given by the graph rule (at lower orders) applied to rooted trees. In summary, each term in the graph expansion of $\gamma^{(1)}_{k_i}/k_i!$ carries the coefficient

$$\frac{(-1)^{|\nu_1(t')|}}{|\mathrm{Aut}(t')|}\,, \quad t' \in \mathcal{T}^{1\bullet}_{k_i+1}\,. \tag{525}$$

Suppose that there are j_i isomorphic subtrees t'_i, $i = 1, \ldots n$ attached to the ω_j vertex. Then, accounting for the $1/j!$ in (524) we obtain the full prefactor for the choice of ω_j, $j \geq 3$, as vertex

$$\prod_{i=1}^{n} \left(\frac{(-1)^{j_i |\nu_1(t'_i)|}}{j_i! |\mathrm{Aut}(t'_i)|^{j_i}} \right). \tag{526}$$

Let $t \in \mathcal{T}_l$ be the graph reassembled from the rooted subtrees t'_i at the vertex with weight ω_j. The total weight is ω_j times the product of the weights of the subtrees and is of the form $\mu(t)$ as in part (ii) of the graph rule. The overall sign $(-)^{|\nu_1(t)|}$, with $|\nu_1(t)|$ the number of internal vertices of t. A straightforward application of the orbit stabilizer theorem shows that the

modulus of (526) equals the symmetry factor of t rooted at our choice of ω_j vertex. As an unrooted graph the overall coefficient is $(-)^{|\nu_1(t)|}/|\mathrm{Aut}(t)|$. There may be several choices of ω_j vertices contributing equally, so the net coefficient for Case 1 is

$$\frac{(-)^{|\nu_1(t)|}}{|\mathrm{Aut}(t)|} \times \#\text{ of } \omega_j \text{ choices with fixed } t. \tag{527}$$

Case 2: middle of an internal line as ω_2 pseudo-vertex. As before, each of the two subtrees attached to ω_2 contributes with coefficient (525). While two subtrees may be distinct or identical, their contribution to the overall symmetry factor will be accounted for by the $1/2!$ prefactor in (524). Again we write $t \in \mathcal{T}_l$ for the graph obtained by reassembling the two subtrees at the ω_2 pseudo-vertex. The overall symmetry factor obtained is that for t rooted at the two ends of the internal line. When reassembled to t via $\partial_\varphi \omega_{n_1-1} \omega_2 \partial_\varphi \omega_{n_2-1} = \omega_{n_1} \omega_2^{-1} \omega_{n_2}$ (with $\omega_{n_1}, \omega_{n_2}$ the weights of the rooted vertices) the overall coefficient is $-(-)^{|\nu_1(t)|}/|\mathrm{Aut}(t)|$. The extra sign accounts for the fact that in the graph rule ω_2^{-1} carries no sign while in (524) the ω_2 term does. There may be several equivalent internal lines in t that are reassembled in this way. The net coefficient for Case 2 then is

$$-\frac{(-)^{|\nu_1(t)|}}{|\mathrm{Aut}(t)|} \times \#\text{ of equivalent internal lines in } t. \tag{528}$$

The full contribution to $\gamma_l/l!$ associated with t is obtained from (524) by summing over the contributions from Case 1 and Case 2 with weight $\mu(t)$ and coefficients (527),(528). This gives

$$\frac{(-)^{|\nu_1(t)|}}{|\mathrm{Aut}(t)|} \times \left(|\nu_1| - |\epsilon_1|\right), \tag{529}$$

where $|\nu_1|$, $|\epsilon_1|$ are the total number of internal vertices and internal lines of t, respectively. For the tree graphs considered the number of external lines and vertices coincide, $|\nu_0| = l = |\epsilon_0|$, so that the Euler relation reduces to $|\nu_1| - |\epsilon_1| = 1$. □

A multi-dimensional version of the above graph rule would similarly relate the vertex functions of a lattice quantum field theory to its connected correlation functions (even at non-zero mean field or source). This is implicit in many text books; a proof can be read off from [53, 16] and also the above derivation carries over. We briefly comment here on this multi-dimensional version in order to highlight that the trees invoked are unrelated to

those in Section 3.3 and 3.4. We denote the standard (unmodified) Legendre transform by $\tilde{\Gamma}[\phi] := \phi \cdot H[\phi] - W[H[\phi]]$, with $W^{(1)}[H[\phi]] = \phi$. Then, $\tilde{\Gamma}^{(1)}[\phi] = H[\phi]$ and the counterpart of (517) reads

$$W^{(1)}\big[\tilde{\Gamma}^{(1)}[\phi]\big] = \phi\,, \quad \tilde{\Gamma}^{(1)}\big[W^{(1)}[H]\big] = H\,. \tag{530}$$

Throughout a superscript (n) denotes n-fold differentiation of a functional of one field with respect to its argument. By repeated differentiation with respect to ϕ or H one obtains in principle mutually equivalent relations between the $\tilde{\Gamma}^{(l)}[\phi]$ (vertex functions in non-zero mean field) and $W^{(l)}[H]$ (cumulants with non-zero source). These coincide essentially with those in the zero-dimensional case (518), just that different lattice sum contractions will remove most of the degeneracies that give rise to non-unit coefficients. That is, in the QFT counterpart of (518) there will be $c_{i_3 \ldots i_{l-1}}$ structurally similar terms (with $W^{(m)}[H[\phi]], \tilde{\Gamma}^{(m)}[\phi]$ replacing ω_m, γ_m, respectively) where the indices in the lattice sums are contracted differently. The graph rule producing these correctly contracted terms in the $\Gamma^{(l)}[\phi]$ expansion invokes the previous tree graphs $\mathcal{T}_l$, but now labeled by lattice points. The external points $x_1, \ldots, x_l$ will be taken distinct but the lattice points summed over in the products of $W^{(k)}_{y_1,\ldots,y_k}$, $k \geq 3$, vertices may coincide. This may occasionally produce coinciding labels for the internal vertices but the tree structure precludes nontrivial automorphisms. A counterpart of the above graph rule can then easily be formulated, see [72, 16] for related Hopf algebraic constructions. Despite the occurrence of labeled tree graphs in this context it is $\tilde{\Gamma}^{(l}[\phi]$, the l-th functional derivative of $\tilde{\Gamma}[\phi]$, that is related to its $W^{(k)}$ counterparts, not the order in a ℓ_{xy} expansion. Performing a κ expansion of both sides of (518)'s multi-dimensional counterpart is of no immediate help in understanding the graph rule underlying Γ's hopping expansion.

Appendix B The Spatial FRG on Friedmann-Lemaître Spacetimes

In this appendix we present a proof of Lemma 6.2.1, together with explicit formulae for the regulator dependent coefficients $q_{1,1}, q_{1,2}, q_{0,1}, q_{0,2}, q_{0,3}$. We begin by recalling the statement of the lemma:

Lemma 6.2.1. *Let $r(x)$ be a generic FRG regulator function as defined in* (446).

(i) The regulator dependent coefficients B_1, B_2, B_3 always satisfy the ratio

$$B_1 : B_2 : B_3 \;=\; -1 : 4 : 3\,, \tag{531}$$

and hence can be expressed in terms of a single regulator dependent constant $q_{0,1}$,

$$B_1 = -6q_{0,1}\,, \quad B_2 = 24q_{0,1}\,, \quad B_3 = 18q_{0,1}\,. \tag{532}$$

(ii) $B_4 + 36q_{0,1} + B_5 = 0$.

(iii) $B_6 = B_7 = B_8$.

Before proceeding to the proof, we note the explicit expressions for $B_1, \ldots, B_8$ from `Mathematica`.

$$B_1 \;=\; -\int_0^\infty d\varrho\, \varrho^2 \frac{\big[r(\varrho^2) - \varrho^2 r^{(1)}(\varrho^2)\big]^2}{4\big[\varrho^2 + r(\varrho^2)\big]^{7/2}}\,, \tag{533}$$

$$\begin{aligned} B_2 \;&=\; -\int_0^\infty d\varrho\, \varrho^2 \frac{\big[r(\varrho^2) - \varrho^2 r^{(1)}(\varrho^2)\big]^2}{2\big[\varrho^2 + r(\varrho^2)\big]^{9/2}} \Big\{ \varrho^4 r^{(2)}(\varrho^2)\big(\varrho^2 + r(\varrho^2)\big) \\ &\quad -\; 4\big(r(\varrho^2) - \varrho^2 r^{(1)}(\varrho^2)\big)\big(5r(\varrho^2) - \varrho^2(2 + 7r^{(1)}(\varrho^2))\big) \Big\}\,, \end{aligned} \tag{534}$$

$$4B_3 \;=\; 3B_2 \tag{535}$$

$$\begin{aligned} B_4 \;&=\; \frac{3}{8}\int_0^\infty d\varrho\, \varrho^2 \frac{\big[r(\varrho^2) - \varrho^2 r'(\varrho^2)\big]^2}{\big[\varrho^2 + r(\varrho^2)\big]^{9/2}} \Big\{ -35r(\varrho^2)^3 \\ &\quad +\; \varrho^2 r(\varrho^2)^2 \Big[42 + 147r'(\varrho^2) + 108\varrho^2 r''(\varrho^2) + 16\varrho^4 r^{(3)}(\varrho^2)\Big] \\ &\quad +\; \varrho^6 \Big[42 r^{(1)}(\varrho^2)^2 + 77 r^{(1)}(\varrho)^3 + 24\varrho^2 r^{(2)}(\varrho^2) - 84\varrho^2 r^{(1)}(\varrho^2) r^{(2)}(\varrho^2) \end{aligned} \tag{536}$$

$$
\begin{aligned}
&+ \quad 16\varrho^4 r^{(3)}(\varrho^2)\Big] \\
&+ \quad \varrho^4 r(\varrho^2)\Big[132\varrho^2 r^{(2)}(\varrho^2) - 21r^{(1)}(\varrho^2)\big(4 + 9r^{(1)}(\varrho^2) + 4\varrho^2 r^{(2)}(\varrho^2)\big) \\
&+ \quad 32\varrho^2 r^{(3)}(\varrho^2)\Big]\Big\} \\
B_5 \;&= \; -\int_0^\infty d\varrho\, \varrho^2 \frac{r(\varrho^2) - \varrho^2 r'(\varrho^2)}{32\big[\varrho^2 + r(\varrho^2)\big]^{9/2}}\Big\{ - 315 r(\varrho^2)^4 \qquad (537) \\
&+ \quad 4\varrho^2 r(\varrho^2)^3\Big[189 + 504 r^{(1)}(\varrho^2) + 606\varrho^2 r^{(2)}(\varrho^2) \\
&+ \quad 192\varrho^4 r^{(3)}(\varrho^2) + 16\varrho^6 r^{(4)}(\varrho^2)\Big] \\
&+ \quad \varrho^8\Big[- 924 r^{(1)}(\varrho^2)^3 - 1155 r^{(1)}(\varrho^2)^4 + 240\varrho^2 r^{(2)}(\varrho^2) \\
&+ \quad 84 r^{(1)}(\varrho^2)^2\big(22\varrho r^{(2)}(\varrho^2) - 1\big) \\
&- \quad 112 r^{(1)}(\varrho^2)\big(3\varrho^2 r^{(2)}(\varrho^2) + 4\varrho^4 r^{(3)}(\varrho^2)\big) \\
&+ \quad 16\varrho^4\big(4\varrho^2 r^{(4)}(\varrho^2) + 20 r^{(3)}(\varrho^2) - 21 r^{(2)}(\varrho^2)^2\big)\Big] \\
&+ \quad 4\varrho^6 r(\varrho^2)\Big[924 r^{(1)}(\varrho^2)^3 + 264\varrho^2 r^{(2)}(\varrho^2) \\
&+ \quad 21 r^{(1)}(\varrho^2)^2\big(31 + 22\varrho^2 r^{(2)}(\varrho^2)\big) \\
&- \quad 14 r^{(1)}(\varrho^2)\big(16\varrho^4 r^{(3)}(\varrho^2) + 78\varrho^2 r^{(2)}(\varrho^2) - 3\big) \\
&+ \quad 8\varrho^2\big(6\varrho r^{(4)}(\varrho^2) + 44 r^{(3)}(\varrho^2) - 21 r^{(2)}(\varrho^2)\big)\Big] \\
&+ \quad 2\varrho^2 r(\varrho^2)^2\Big[- 2121 r^{(1)}(\varrho^2)^2 + 6\big(270\varrho^2 r^{(2)}(\varrho^2) - 7\big) \\
&- \quad 14 r^{(1)}(\varrho^2)\big(16\varrho^4 r^{(3)}(\varrho^2) + 144\varrho^2 r^{(2)}(\varrho^2) + 87\big) \\
&+ \quad 8\varrho^2\big(12\varrho^2 r^{(4)}(\varrho^2) + 116 r^{(3)}(\varrho^2) - 21 r^{(2)}(\varrho^2)^2\big)\Big]\Big\}\,,
\end{aligned}
$$

and

$$
\begin{aligned}
B_6 \;&= \; \int_0^\infty d\varrho\, \varrho^2 \frac{r(\varrho^2) - \varrho^2 r'(\varrho^2)}{2\big[\varrho^2 + r(\varrho^2)\big]^{7/2}}\Big\{ - 3 r(\varrho^2) + \varrho^2\big(2 + 5 r^{(1)}(\varrho^2)(\varrho^2)\big)\Big\}\,, \qquad (538) \\
B_7 \;&= \; \int_0^\infty d\varrho\, \varrho^2 \frac{r(\varrho^2) - \varrho^2 r'(\varrho^2)}{4\big[\varrho^2 + r(\varrho^2)\big]^{9/2}}\Big\{ - 9 r(\varrho^2)^2 \qquad (539) \\
&+ \quad 2\varrho^2 r(\varrho^2)\Big[11 + 20 r^{(1)}(\varrho^2) + 10\varrho^2 r^{(2)}(\varrho^2)\Big]
\end{aligned}
$$

$$+ \quad \varrho^4\Big[20\varrho^2 r^{(2)}(\varrho^2) - 5r^{(1)}(\varrho^2)\big(6 + 7r^{(1)}(\varrho^2)\big) - 4\Big]\Big\}\,,$$

$$B_8 \;=\; B_6\,. \tag{540}$$

Proof. (Lemma 6.2.1)

(i) The ratio $B_2 : B_3 = 4 : 3$ is clearly manifest in (535), so it remains to show

$$4B_1 + B_2 = 0\,. \tag{541}$$

Indeed, it follows by direct computation that

$$\begin{aligned} 4B_1 + B_2 \;&=\; \frac{1}{2}\int_0^\infty d\varrho\,\frac{\partial}{\partial\varrho}\left\{\frac{\varrho^3 r(\varrho^2)^2 - 2\varrho^5 r(\varrho^2)r^{(1)}(\varrho^2) + \varrho^7 r^{(1)}(\varrho^2)^2}{\big[\varrho^2 + r(\varrho^2)\big]^{7/2}}\right\} \\ &=\; \lim_{\varrho\to\infty}\frac{\varrho^3 r(\varrho^2)^2 - 2\varrho^5 r(\varrho^2)r^{(1)}(\varrho^2) + \varrho^7 r^{(1)}(\varrho^2)^2}{2\big[\varrho^2 + r(\varrho^2)\big]^{7/2}}\,. \end{aligned} \tag{542}$$

By Property **Reg (iii)** of the regulator function $R_k(t, p^2)$, it follows that $r(\varrho^2)$ and its derivatives must approach zero as $\varrho \to \infty$ faster than any polynomial in ϱ. Thus (542) vanishes, i.e. $4B_1 + B_2 = 0$, establishing Lemma 6.2.1*(i)*.

(ii) Similarly, one finds

$$\begin{aligned} B_4 + 36q_{0,1} + B_5 \;&=\; \int_0^\infty d\varrho\,\frac{\partial}{\partial\varrho}\Bigg\{\frac{\varrho^3}{32\big[\varrho^2 + r(\varrho^2)\big]^{11/2}}\Big[5r(\varrho^2)^4 \\ &-\; 4\varrho^2 r(\varrho^2)^3\big(22 + 27r^{(1)}(\varrho^2) + 36\varrho^2 r^{(2)}(\varrho^2) + 8\varrho^4 r^{(3)}(\varrho^2)\big) \\ &+\; \varrho^8\Big(112r^{(1)}(\varrho^2)^3 + 105r^{(1)}(\varrho^2)^4 - 16\varrho^4 r^{(2)}(\varrho^2)^2 \\ &+\; 4r^{(1)}(\varrho^2)^2[3 - 28\varrho^2 r^{(2)}(\varrho^2)] + 32\varrho^2 r^{(1)}(\varrho^2)[r^{(2)}(\varrho^2) + \varrho^2 r^{(3)}(\varrho^2)]\Big) \\ &+\; 2\varrho^4 r(\varrho^2)^2\Big(6 + 153r^{(1)}(\varrho^2) - 88\varrho^2 r^{(2)}(\varrho^2) \\ &-\; 8\varrho^2[r^{(2)}(\varrho^2)^2 + 4r^{(3)}(\varrho^2)] + 16r^{(1)}(\varrho^2)[9 + 8\varrho^2 r^{(2)}(\varrho^2) + \varrho^4 r^{(3)}(\varrho^2)]\Big) \\ &-\; 4\varrho^6 r(\varrho^2)\Big(77r^{(1)}(\varrho^2)^3 + 2r^{(1)}(\varrho^2)^2[39 + 14\varrho^2 r^{(2)}(\varrho^2)] \\ &+\; 8\varrho^2 r^{(2)}(\varrho^2)(\varrho^2) + 8\varrho^2[r^{(2)}(\varrho^2)^2 + r^{(3)}(\varrho^2)] \\ &-\; 2r^{(1)}(\varrho^2)[8\varrho^2 r^{(3)}(\varrho^2) + 36\varrho^2 r^{(2)}(\varrho^2) - 3]\Big)\Big]\Bigg\}\,, \end{aligned} \tag{543}$$

which vanishes for a generic regulator function r due to the same reason as (542). This establishes Lemma 6.2.1*(ii)*.

(iii) As above, direct computation yields

$$B_6 - B_7 \;=\; -\int_0^\infty d\varrho\, \frac{\partial}{\partial \varrho}\Big\{ \frac{5\varrho^3\big[r(\varrho^2) - \varrho^2 r^{(1)}(\varrho^2)\big]^2}{4\big[\varrho^2 + r(\varrho^2)\big]^{7/2}} \Big\} = 0\,. \tag{544}$$

Together with (540) this completes our proof of Lemma 6.2.1.

□

We end this appendix with a summary of the expressions for the regulator dependent coefficients in (471).

$$q_{1,1} \;=\; \frac{1}{12}\int_0^\infty d\varrho\, \varrho^2 \frac{\big[r(\varrho^2) - \varrho^2 r^{(1)}(\varrho^2)\big]^2}{\big[\varrho^2 + r(\varrho^2)\big]^{5/2}}\,, \quad q_{1,2} = -\int_0^\infty d\varrho\, \varrho^2 \frac{r(\varrho^2) - \varrho^2 r^{(1)}(\varrho^2)}{\big[\varrho^2 + r(\varrho^2)\big]^{3/2}}\,, \tag{545}$$

$$q_{0,1} \;=\; \frac{3}{2}\int_0^\infty d\varrho\, \varrho^2 \frac{\big[r(\varrho^2) - \varrho^2 r'(\varrho^2)\big]^2}{\big[\varrho^2 + r(\varrho^2)\big]^{7/2}}\,, \quad q_{0,2} = -\frac{B_5}{12}\,,$$

$$q_{0,3} \;=\; \int_0^\infty d\varrho\, \varrho^2 \frac{r(\varrho^2) - \varrho^2 r'(\varrho^2)}{2\big[\varrho^2 + r(\varrho^2)\big]^{7/2}}\Big\{ -3r(\varrho^2) + \varrho^2\big(2 + 5r^{(1)}(\varrho^2)(\varrho^2)\big)\Big\}\,. \tag{546}$$

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