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Large Distance Expansion in the Schrödinger Representation of Quantum Field Theory

by

Marcos Donizeti Rodrigues Sampaio

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ABSTRACT

Large Distance Expansion in the Schrödinger Representation of Quantum Field Theory

Marcos Donizeti Rodrigues Sampaio

This thesis is concerned with an approach to Quantum Field Theory in which the states are constructed from their large distance behaviour. The logarithm of the vacuum functional is expandable as a local quantity in any quantum field theory in which the lightest physical particle has a non-zero mass. This local expansion satisfies its own form of the Schrödinger equation from which its coefficients can be determined. We illustrate for ϕ_{1+1}^4 -theory that our local expansion incorporates correctly the short distance behaviour as contained in the counterterms of the Hamiltonian. A Feynman diagram expansion of the vacuum functional is also presented. The amplitudes are calculated and their large distance expansion are in good agreement with our semi-classical solution of the Schrödinger equation. Some applications of this formalism to the study of the Schrödinger functional are also suggested.

Declaration

This thesis is the result of research carried out between May 1994 and May 1997. The work presented in this thesis has not been submitted in fulfilment of any other degree or professional qualification.

No claim of originality is made for chapters 1, 2 and 3, except for section 3.4 which was formulated in collaboration with Dr. Paul Mansfield, and part of section 3.5, in collaboration with Dr. Jiannis Pachos. Chapter 4 arose from collaboration between myself, Dr. Paul Mansfield and Dr. Jiannis Pachos resulting in the publication *Short Distance Properties from Large Distance Behaviour*, *DTP – 96/65* which also contains results from my independent work presented in chapter 5. Chapter 6 contains my independent work concerning the Schrödinger functional. The computer program presented in the appendix *B* resulted from a cooperative work with Dr. Jiannis Pachos.

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Dedicated to Pascale

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Introduction

It is clear that quantum field theory (QFT) is the most successful paradigm from both a theoretical and experimental standpoint. Symmetry principles have always been the main ingredient in formulating quantum field theories. The Standard Model of particle physics is the most prominent example. It is also a consensus that we must go beyond QFT to find the answer for the problem the quantisation of gravity, for example. A new framework, richer in symmetries such as String Theory, will have to be exploited, presumably having QFT as a low energy limit. This does not mean at all that we have exhausted QFT as a source of information about physical phenomena. To the contrary, there are many unsolved problems in physics which should be clarified by QFT in its most elementary setting. For example, in QCD, perhaps our most complete field theory, there remains to be developed an analytical framework to control its infra-red sector where we cannot use perturbation theory in the couplings. This is essential to understand the mechanism responsible for confinement and other low-energy phenomena in QCD so that it can be crowned as the theory of strong interactions.

However, the arsenal of non-perturbative methods is scarce and most of the information in the non-perturbative limit comes from numerical computations by formulating the theory on a lattice. Analytical approaches usually provide more physical insight than numerical simulations and often the interplay between the two approaches is very profitable.

The Schrödinger representation in QFT and the language of wave functionals have given encouraging results as an analytical framework to study physics beyond perturbation theory. For example, Mansfield [1] showed that within a continuum strong coupling expansion of the Yang-Mills vacuum functional, the leading order term leads to confinement via a kind of dimensional reduction resulting from the local nature of the logarithm of the vacuum functional. This has been generalised in [24] to the case of the Wheeler-De

Witt equation to look for a new phase in quantum gravity beyond the Planck scale.

Generally speaking, it was shown in [2] that, at large distances, the vacuum functional of any quantum field theory whose lightest physical particle is non-zero undergoes a significant simplification: for slowly varying fields its logarithm becomes a local functional of the fields. It is local in the sense that it reduces to a single spatial integral of a sum of terms, each of which is constructed from the field and a finite number of derivatives evaluated at the same spatial point. This expansion is expected to converge for fields that vary slowly on the scale of the lightest particle in the theory which it describes. This is in contrast to a very non-local expression which we would get if it was evaluated for more rapidly varying fields.

Although this approach has been shown to be successful in studying the confining properties of Yang-Mills theories since the first term in the local expansion exhibits confinement, in order to evaluate physical quantities we should compute more coefficients in the local expansion. To calculate the so called low-hadron spectrum, which involves heavier particles and therefore more rapidly varying fields, the local expansion can still be useful. That is because by exploiting the analyticity properties of the vacuum functional under complex scalings, it is possible to reconstruct it for arbitrary fields.

The coefficients of the local expansion are, in principle, determined by the Schrödinger equation. However, care must be exercised because this equation depends explicitly on short distance effects via an ultraviolet cut-off whereas the local expansion is valid only for fields characterised by large length scales. Again analyticity properties of the Schrödinger equation enable us to construct a version of this equation satisfied by the local expansion. This reduces the eigenvalue problem of the Hamiltonian to a set of algebraic equations. For theories that are massive at the classical level these equations may be solved semi-classically. As a bonus, this set of equations offers the possibility of solution within a new scheme which holds for theories that are massless at the classical level, but acquire mass quantum mechanically. This new approach to the solution does not rely on the smallness of the coupling constant and hence offers the possibility of solution beyond perturbation theory.

This thesis is organised as follows: In chapter 1, we give an overview of the Schrödinger representation in QFT and present a few examples. In chapter 2, we demonstrate the sim-

plification of the vacuum functional at large distances and show how it can be reconstructed from its large distance, local expansion. We construct the Schrödinger equation satisfied by the local expansion and discuss the approaches to its solution in chapter 3. Chapters 4, 5 and 6 contain the main results of this thesis. In chapter 4 we show for ϕ_{1+1}^4 -theory that the short distance behaviour contained in the counterterms of the Hamiltonian is correctly reproduced by our approach to the Schrödinger equation in which the vacuum state is constructed from its large distance expansion. In chapter 5, we obtain the vacuum functional of ϕ_{1+1}^4 -theory by using its Feynman diagram interpretation. We evaluate some amplitudes and find out that, in the limit of slowly varying fields, they are in good agreement with the results which we have obtained by solving the Schrödinger equation. In chapter 6, we argue that the Schrödinger functional can be locally expanded for small time, even if the theory is massless. We also illustrate how we could reconstruct the Schrödinger functional from its small time expansion. Finally we obtain the leading order short time behaviour of the Yang-Mills-Schrödinger functional within a local expansion in the fields. In appendix A, we study the analyticity properties of the kinetic term in the Schrödinger equation and in appendix B we present a computer programme which was useful to generate the algebraic equations that determine the coefficients of the local expansion. Throughout this thesis, we have adopted the unit system such that $\hbar = c = 1$, except where they are explicitly written.

Chapter 1

The Schrödinger Representation in Quantum Field Theory

1.1 Introduction

The Schrödinger Representation in Quantum Field Theories (SRQFT) is a natural extension of ordinary Quantum Mechanics in which we start out with a Hamiltonian operator and canonically quantise by postulating commutation relations between the coordinate operators and their conjugate momenta. The coordinate Schrödinger representation is achieved by representing the diagonal position operator with its eigenvalues and using a differential representation of the commutators by replacing the conjugate momenta with derivatives. Coordinate representations of state vectors are called wave functions. The Schrödinger equation becomes a differential equation whose solutions, the eigenfunctions of the Hamiltonian differential operator, represent possible states of the system. The dynamics thus resides in the states rather than in the field operators .

For a field theory in the Schrödinger representation we have, in principle, only to substitute the word *function* by *functional*. Differential representations for the canonical commutators are achieved by replacing the conjugate momenta with functional derivatives. Coordinate representations of the state vectors are wave functionals. The Schrödinger equation becomes a functional differential equation whose solutions represent possible states of the system. In this sense, together with the Path Integral formalism, the SRQFT constitutes a functional representation of field theory.

Although the SRQFT is an old concept, only recently it has been used as a tool to work out field theoretic results instead of the Green's function method for Fock space matrix

elements of Heisenberg picture operators. This is partially due to technical complications that one has to face. Solving the (Schrödinger) functional differential equation for a field theory can be a highly non-trivial task, in the first place. Furthermore, in contrast with the Heisenberg picture, we miss the explicit Lorentz covariance. This apparent lack of Lorentz covariance stems from the fact that quantum states are represented by wave functionals of the fields on space-like surfaces, the Schrödinger equation describing the evolution of the wave functional between successive surfaces. Thus, while the field configurations on that surface carry the representations of internal symmetry groups, as well as isometry groups of the surfaces themselves, the symmetries of the background space-time metric, such as the Poincaré group, are affected. This is because the latter involves motions or distortions of the surfaces in the space-time whereas the fields defined thereon generally carry no information about the surface location or orientation with respect to the background space-time¹.

Another difficulty in using a wave functional description of quantum field theories lies in describing their renormalisation properties. Indeed, infinities can be more easily isolated within the framework of causal Green's functions in the Heisenberg formalism. The renormalisation features of the SRQFT were firstly addressed in a seminal work by Symanzik [5] in which the Schrödinger picture was established in a mathematically well-defined way for the scalar ϕ^4 theory in $(3+1)$ -dimensions. He showed, in perturbation theory, that the wave functional defined through a functional integral is finite as any ultraviolet cut-off is removed if, in addition to the usual ones, (two) additional counterterms are introduced in the Lagrangian. This results from additional infinities that occur owing to the presence of an extra boundary (at $t = 0$), where the interpretation of the wave functional as a probability amplitude is given.

For time-dependent problems, the renormalisation was firstly studied in [23] in the context of time-dependent variational equations for Gaussian trial wave functionals, envisaging cosmological applications.

Despite the difficulties appearing from the technicalities mentioned above, there are

¹A different formulation of the problem which aimed at establishing a covariant way to quantise quantum field theory in the Schrödinger representation was originally proposed by Dirac [56] using parametrised field theory (see also [26]). The basic idea was to raise the status of the space-time coordinates (called embedding variables) to dynamical variables. In this sense, the wave functional turns out to depend on the field configurations on the surface and the embeddings X^α . Then one can talk about symmetry groups that involve motions of the three-surfaces themselves.

many problems, especially those involving changes in the ground state properties, in which our intuitive understanding is better served in a wave functional Hamiltonian framework. For instance, in the case of bosonic fields, the Schrödinger representation is a direct generalisation from ordinary quantum mechanics to the infinite number of degrees of freedom that constitutes a field. This suggests the possibility of using the physical/mathematical intuition acquired in quantum mechanics to analyse field theoretic problems². For example, if we recall that while the Green's function formalism contains all the information to calculate objects like transition rates, S-matrix elements, etc. of systems in equilibrium (where the initial data are superfluous), it is in the Schrödinger representation that we can deal with the problem of following the evolution of a system in time from a definite initial configuration (a pure or mixed state)[18]. This concerns many cosmological problems such as the time evolution of the inflation-driving-field and details of (thermal) phase transitions which might have given rise to structures like cosmic strings [10],[12],[8].

The SRQFT is the ideal framework to describe anomalies and large gauge transformations [37]. In the case of anomalies, the basic idea is to consider the Schrödinger wave functional represented as a path integral and detect the anomaly in the non-invariant measure. Alternatively, after properly defining the action of the transformation operators upon the wave functional, one can study their commutators and find out about the appearance of anomalous terms [33].

In a formulation of quantum field theory similar to quantum mechanics, one could think of applying techniques which we learned from the latter to the former. The variational method is the obvious candidate. The Gaussian variational method in the functional Schrödinger picture has shown to be a good guide for the study of some non-perturbative aspects of scalar and fermionic theories as well as for the description of quantum scalar fields in an external electromagnetic background [11],[12],[21],[22]. For example, in [11] it was shown that the Gaussian approximation gives better results than the $1/N$ approximation, N being the number of fermion flavours, in describing the dynamical breaking of parity (chiral) symmetry in the $(2 + 1)$ -dimensional Thirring Model. Also, in non-equilibrium (finite temperature) quantum field theory, which is important to study the early universe cosmology, the density matrix ρ describing a system in a mixed state satisfies the quantum Liouville-Von Neumann (LVN) equation $d\rho/dt = i[\rho, H]$ if we assume an

²For a review, see [15].

isoentropic time evolution with the time dependence governed by the Hamiltonian H (for example, via a time-dependent metric). This equation can only be solved for problems that are described by quadratic Hamiltonians but for more general Hamiltonians, observing that the LVN equation can be derived from a variational principle [57], a Gaussian approximation for the density matrix can be used as an approximation. The resulting variational equations lead to a set of self consistent equations that unlike perturbation theory, reflect some of the non-linearities of the full quantum theory [58],[59],[8].

The development of an analytical non-perturbative framework to study the low energy phenomena in non-abelian gauge theories is highly desirable. Quantum gauge field theories have been successfully tested for high energy phenomena, where the interaction can be treated in a perturbative way (and a linearisation can be carried out) within the framework of path integrals, for example. Asymptotic freedom enable us to perform quantitative perturbative calculations of observables which are sensitive to the short distance (or large momentum transfers) structure of QCD. However, at large distances the coupling becomes large (infrared slavery) and the perturbative expansion senseless. Consequently, perturbation theory fails to reproduce the low energy phenomena. Among them, we can mention the quark confinement problem and chiral symmetry breaking in QCD (which are the mechanisms responsible for the spectrum of the low lying hadron states). Obtaining a consistent picture of the vacuum of strongly coupled gauge theories constitutes one of the major problems in quantum field theory.

On the other hand, the arsenal of non-perturbative methods is very limited. One of them is the numerical approach of Wilson's Lattice Gauge Theory, which has provided considerable progress in the matter. The great advantage of this formalism is that the theory is quantised in a gauge invariant way. The price to be paid is that the continuous nature of the space-time is spoilt and the connection with continuum field theory is established only numerically. The idea is to regularise the theory by discretising the Euclidean space time to a cubic lattice with periodic boundary conditions and solve the resulting integrals by Monte Carlo methods [74],[19]. Lattice calculations have given evidence that QCD and Yang-Mills theories are confining: a non-zero value of the string tension can be numerically calculated. However, the available computational power has limited a complete analysis based on a lattice field theory. Moreover, to get some insight into the physics behind the low-energy phenomena, one should develop analytical methods, capable of solving the low

energy sector of QCD starting from first principles.

The Hamiltonian formulation of Yang-Mills theory has given profitable contributions in this sense although the exact solution of its vacuum functional is still lacking. The functional differential equation satisfied by the Yang-Mills vacuum functional is very hard to solve, partially because of its non-abelian character. However, approximate vacuum functionals have been suggested, valid in the strong-coupling limit or long-wavelength configurations [46],[1],[43],[44] (which is the domain where the low hadron-spectrum originates) as well as interpolating forms between long and short-wavelength configurations [41]. They find support in strong coupling expansions in the lattice where the computations can be more satisfactorily made in lower dimensions (e.g. in $2+1$ -dimensions), and the results extrapolated to the physical dimensions via arguments of dimensional reduction [1],[60],[61],[62].

Successfully applied to some problems in quantum field theory, the variational approach presents more difficulties when applied to gauge fields. It is very hard to find a set of wave functionals which are both gauge invariant and amenable to analytic calculation. It can actually be shown that it is not possible to write a Gaussian wave functional which satisfies the constraint of gauge invariance although some alternatives have been suggested to remedy the problem [13].

The pioneer work on the Schrödinger functional equation for Yang-Mills theories was done by Feynman [16]. He considered $(2+1)$ -dimensional Yang-Mills theories with a view to explaining the confinement of gluons. This was among his last important papers. For a review of his paper, see also [17]. He considerably simplifies the problem of QCD to set grounds for his arguments. The full problem involves 104 functions: six flavours of quarks, each with three colours, each of which are represented by a Dirac spinor with four components plus thirty-two functions representing eight gluon vector fields each with four components. The first simplification was to restrict to gluons only and ignore quarks. As Feynman says, there are indications, from studies of asymptotic freedom and related matters, that in the confinement problem the effects of quarks, if anything, work slightly against the greater effects of gluons. The other simplification was to work with $SU(2)$ instead of the $SU(3)$ gauge group. This is motivated by the fact that this simplified model does present the feature of colour confinement, and a sufficiently intricate and interesting

vacuum structure. This reduces the problem to three gluon fields which amounts to 6 different functions if we work in the temporal gauge, in which the time-like component of the potential is set to zero, and in $(2 + 1)$ -dimensions. About whether such simplification is realistic, we also respond using Feynman's words: "... the ease of visualisation is so much greater that I think it is worth the risk!". To summarise the results, Feynman gave qualitative arguments in support of the existence of a finite gap in the energy spectrum of the Yang-Mills Hamiltonian above the ground state vacuum, so that the first excited state is a massive excitation, presumably a glueball. This is intrinsically connected to the non-abelian character of the theory. In the case of QED, such a mass gap can be made arbitrarily small so that the excitation is a massless "gluon" (photon).

As discussed by Jackiw in [15] we can heuristically put the problem as follows: in quantum mechanics, the energy eigenfunctions $\Psi_E(q)$ for a system with an energy gap differ from those where there is no gap in the sense that, in the latter case, the dynamical variable q can become arbitrarily large. This becomes clear if you recall that the free motion of a particle in an unbounded region possesses a continuous spectrum (there is no gap and thus the energy can be as close as you want to the fundamental state) whereas if the region is bounded (for instance, a double well), and therefore q is limited, a gap exists and the spectrum is discrete. In field theory we observe that, in electrodynamics, a long wavelength vector potential corresponding to a low energy photon with energy arbitrarily close to the vacuum exists. Feynman argues and presents some rough calculations to prove that, for non-abelian gauge theories, such "large configurations" are either gauge equivalent to "small" ones, or damped by the magnetic potential energy. On more mathematical grounds, this problem was approached by Atiyah, Singer and Hitchin in [63], where they study the metric on the space of Yang-Mills configurations.

Another important field of application of SRQFT is quantum gravity. Since Quantum General Relativity is non-renormalisable at perturbative level, one has to develop non-perturbative methods provided the theory is viable at all. Remarkable progresses have been achieved in canonical quantum gravity in recent years by using the Schrödinger picture. For instance, a class of exact solutions for the constraint equations (Wheeler-De Witt equation) has been calculated [24],[25],[64].

In the next sections, we present an introduction to the formalism of SRQFT illustrated

with a few examples and discuss some of its applications.

1.2 Scalar Fields

For bosonic fields, the functional Schrödinger representation is a simple generalisation of quantum mechanics. Fermionic and gauge fields theories are more complicated than scalar field theories because of the anticommutators and gauge degrees of freedom, respectively. The Lagrangian density for the scalar field ϕ reads

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi - U(\phi) \equiv \frac{1}{2} (\dot{\phi}^2 - (\nabla\phi)^2) - U(\phi), \quad (1.1)$$

where the dot represents differentiation with respect to time. The field canonically conjugate to ϕ is

$$\frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \dot{\phi} = \pi \quad (1.2)$$

and then the Hamiltonian density becomes

$$\mathcal{H} = \pi \dot{\phi} - \mathcal{L} = \frac{1}{2} \dot{\phi}^2 + \frac{1}{2} (\nabla\phi)^2 + U(\phi) \quad (1.3)$$

which enables us to write the Hamiltonian as

$$H = \int \mathcal{H} d^3\mathbf{x} = \int d^3\mathbf{x} \left(\frac{1}{2} \pi^2 + \frac{1}{2} (\nabla\phi)^2 + U(\phi) \right) \quad (1.4)$$

By complete analogy to quantum mechanics, we can canonically quantise the theory by treating the fields as operators and imposing the equal-time commutation relations:

$$\begin{aligned} [\hat{\phi}(\mathbf{x}, t), \hat{\pi}(\mathbf{x}', t)] &= i\delta^3(\mathbf{x} - \mathbf{x}'), \\ [\hat{\phi}(\mathbf{x}, t), \hat{\phi}(\mathbf{x}', t)] &= 0, \\ [\hat{\pi}(\mathbf{x}, t), \hat{\pi}(\mathbf{x}', t)] &= 0. \end{aligned} \quad (1.5)$$

In the coordinate Schrödinger representation, we take the basis-vectors of the state vector space to be the eigenstates of the field operator $\hat{\phi}$ on a fixed time hypersurface (t , say) with eigenvalues $\varphi(\mathbf{x})$, namely ³

$$\hat{\phi}(x)|\varphi(\mathbf{x})\rangle = \varphi(\mathbf{x})|\varphi(\mathbf{x})\rangle \quad (1.6)$$

³Notice that the set of field eigenvalues is independent of the value of t labelling the hypersurface.

where now φ is an ordinary scalar function and the eigenstates $|\varphi\rangle$ satisfy the usual orthonormality and completeness relation:

$$\begin{aligned}\langle\varphi(\mathbf{x})|\varphi'(\mathbf{x})\rangle &= \delta[\varphi - \varphi'] \\ \int \mathcal{D}\varphi |\varphi(\mathbf{x})\rangle\langle\varphi(\mathbf{x})| &= \hat{1}\end{aligned}\quad (1.7)$$

The coordinate Schrödinger representation of a generic state $|\Psi\rangle$ is the wave functional $\Psi[\varphi]$, a functional of the eigenvalue φ

$$\Psi[\varphi] = \langle\varphi|\Psi\rangle \quad (1.8)$$

and an inner product is defined through functional integration, that is

$$\langle\Psi_1|\Psi_2\rangle = \int \mathcal{D}\varphi \Psi_1^*[\varphi]\Psi_2[\varphi]. \quad (1.9)$$

Also

$$\begin{aligned}\hat{\phi} &\longrightarrow \varphi(\mathbf{x}) \\ \hat{\pi} &\longrightarrow -i\frac{\delta}{\delta\varphi(\mathbf{x})}\end{aligned}\quad (1.10)$$

constitutes a functional differential representation of the equal time commutators. The action of any operator composed by the canonical variables on the state $|\Psi\rangle$ is

$$\mathcal{O}(\hat{\phi}, \hat{\pi})|\Psi\rangle \mapsto \mathcal{O}\left(\varphi, \frac{1}{i}\frac{\partial}{\partial\varphi}\right)\Psi[\varphi] \quad (1.11)$$

and the dynamical equation is the functional Schrödinger equation for time dependent functionals

$$H\left(\varphi, \frac{1}{i}\frac{\partial}{\partial\varphi}\right)\Psi[\varphi] = i\frac{\partial}{\partial t}\Psi[\varphi] \quad (1.12)$$

which, for time independent Hamiltonians, a separation of variables trivialises the time dependence $\Psi_t[\varphi] = e^{-iEt}\Psi[\varphi]$ and we are left with the functional eigenvalue problem

$$H\left(\varphi, \frac{1}{i}\frac{\partial}{\partial\varphi}\right)\Psi[\varphi] = E\Psi[\varphi]. \quad (1.13)$$

For the free case, $U(\phi) = \frac{1}{2}m^2\phi^2$ and the Hamiltonian can be written as

$$H = \frac{1}{2} \int d^3\mathbf{x} \left(\frac{\delta^2}{\delta\varphi(\mathbf{x})\delta\varphi(\mathbf{x})} + \varphi(\mathbf{x})(-\nabla^2 + m^2)\varphi(\mathbf{x}) \right). \quad (1.14)$$

which has the same structure as the simple harmonic oscillator. We can try to solve it for the ground state wave functional and therefore assume that the functional has no nodes

and is positive everywhere. Thus we may expect that the ground state is described by a Gaussian wave functional

$$\Psi_0[\varphi] = \mathcal{N} e^{-\frac{1}{2} \int d^3\mathbf{x} d^3\mathbf{y} \varphi(\mathbf{x}) G(\mathbf{x}, \mathbf{y}) \varphi(\mathbf{y})} \quad (1.15)$$

which substituted back into (1.14) yields ⁴

$$\begin{aligned} \int d^3\mathbf{x} d^3\mathbf{y} \frac{1}{2} \left(G(\mathbf{x}, \mathbf{x}) \delta(\mathbf{x} - \mathbf{y}) - \varphi(\mathbf{x}) G^2(\mathbf{x}, \mathbf{y}) \varphi(\mathbf{y}) + \varphi(\mathbf{x}) (-\nabla^2 + m^2) \varphi(\mathbf{x}) \right) \Psi_0[\varphi] \\ = E_0 \Psi_0[\varphi] \end{aligned}$$

We arrive at a set of equations for E_0 and G , namely

$$\begin{aligned} G^2(\mathbf{x}, \mathbf{y}) &= (-\nabla^2 + m^2) \delta(\mathbf{x} - \mathbf{y}) \\ E_0 &= \frac{1}{2} \text{Tr} G \equiv \frac{1}{2} \int d^3\mathbf{x} G(\mathbf{x}, \mathbf{x}) \end{aligned} \quad (1.16)$$

The equations above can be easily solved by using the Fourier transformation method which results

$$\begin{aligned} G(\mathbf{x} - \mathbf{y}) &= \frac{1}{(2\pi)^3} \int d^3\mathbf{p} e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \sqrt{\mathbf{p}^2 + m^2} \\ E_0 &= \int d^3\mathbf{x} \frac{1}{(2\pi)^3} \int d^3\mathbf{p} \frac{1}{2} \sqrt{\mathbf{p}^2 + m^2} \end{aligned} \quad (1.17)$$

So, the vacuum wave functional for the scalar theory is given by 1.15 with G calculated above and E represents the well-known zero-point energy of the free scalar field. In the momentum space, it reads

$$\Psi_0[\tilde{\varphi}] = \mathcal{N}' e^{-1/2 \int d^3\mathbf{p} / (2\pi)^3 \tilde{\varphi}(\mathbf{p}) \tilde{\varphi}(-\mathbf{p}) \omega_p} \quad (1.18)$$

where $\omega_p = \sqrt{\mathbf{p}^2 + m^2}$. The normalisation constant \mathcal{N}' is determined by the usual requirement $\int \mathcal{D}\tilde{\varphi} \Psi_0^*[\tilde{\varphi}] \Psi_0[\tilde{\varphi}] = 1$ with $\mathcal{D}\tilde{\varphi} = \prod_p d\tilde{\varphi}_p / (2\pi)^3$ which gives

$$\mathcal{N}' = \prod_p \left(\frac{\omega_p}{\pi} \right)^{1/4} \quad (1.19)$$

In complete analogy with quantum mechanics, we can define creation and annihilation operators

$$\begin{aligned} a(\mathbf{p}) &= \frac{1}{\sqrt{2}} \int d^3\mathbf{x} e^{+i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \left(\omega^{1/2}(\mathbf{p}) \hat{\phi}(\mathbf{x}) + i\omega^{-1/2}(\mathbf{p}) \hat{\pi}(\mathbf{x}) \right) \\ a^\dagger(\mathbf{p}) &= \frac{1}{\sqrt{2}} \int d^3\mathbf{x} e^{-i\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \left(\omega^{1/2}(\mathbf{p}) \hat{\phi}(\mathbf{x}) - i\omega^{-1/2}(\mathbf{p}) \hat{\pi}(\mathbf{x}) \right) \end{aligned} \quad (1.20)$$

⁴The bilocal kernel $G(\mathbf{x}, \mathbf{y})$ regularises the product of two functional derivatives at the same spatial point in 1.14 which is ill defined.

satisfying $[a(\mathbf{p}), a^\dagger(\mathbf{p}')] = (2\pi)^3 \delta(\mathbf{p} - \mathbf{p}')$. The Hamiltonian written in these variables reads

$$H = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \omega(\mathbf{p}) a^\dagger(\mathbf{p}) a(\mathbf{p}) + \frac{1}{2} \int \frac{d^3\mathbf{p}}{(2\pi)^3} G(\mathbf{p}, \mathbf{p}) \quad (1.21)$$

with $G(\mathbf{p}, \mathbf{p}') = \omega(\mathbf{p})(2\pi)^3 \delta^3(\mathbf{p} - \mathbf{p}')$.

Excited states can be constructed by applying the ladder operators on the ground state wave functional. Their functional coordinate representation is achieved by using the functional derivative representation of the momentum operator resulting

$$\begin{aligned} a(\mathbf{p}) &= \frac{1}{\sqrt{2}} \int d^3\mathbf{x} e^{+i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \left(\omega^{1/2}(\mathbf{p})\varphi(\mathbf{x}) + i\omega^{-1/2}(\mathbf{p}) \frac{\delta}{\delta\varphi(\mathbf{x})} \right) \\ a^\dagger(\mathbf{p}) &= \frac{1}{\sqrt{2}} \int d^3\mathbf{x} e^{-i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \left(\omega^{1/2}(\mathbf{p})\varphi(\mathbf{x}) - i\omega^{-1/2}(\mathbf{p}) \frac{\delta}{\delta\varphi(\mathbf{x})} \right) \end{aligned} \quad (1.22)$$

with the property $a(\mathbf{p})\Psi_0[\varphi] = 0$. The first excited state is $\Psi_1[\varphi] = \mathcal{N}' a^\dagger(\mathbf{p}_1)\Psi_0[\varphi]$, which represents a state with one scalar particle of mass m , momentum \mathbf{p}_1 and energy ω_{p_1} .

As we have seen, the functional Schrödinger representation of the scalar field has the same structure as quantum mechanics. In principle, one could obtain information about the quantum field theory using similar techniques we find in quantum mechanics. However, unlike the free case, for interacting theories the Schrödinger equation cannot be solved in a closed form in general. As the variational method in quantum mechanics provides a very good approximation for certain problems, one expect to be able to apply it to quantum field theories as well. The scheme is as follows: the dynamical equations are obtained as the condition that some quantity be stationary against arbitrary variations. This can be implemented approximately by choosing the quantities to be varied to have a specific form, e.g. a Gaussian wave function(al), parametrised by certain unknown parameters which will be varied. In this way one might arrive at a set of self consistent equation, solvable for those parameters.

1.3 Variational Approximations in the Schrödinger Picture

Action principles rule the dynamics of the theories which they govern. For example, in classical mechanics the equations of motion are derived by Hamilton's variational principle which requires stationarising the classical action $S_{clas} = \int dt L(\dot{q}, q)$, such that $\delta S_{clas}/\delta q(t) = 0$ with the variation $\delta q(t)$ vanishing at the endpoints that define the action. The quantum analogue is called *Dirac's action principle*. It instructs to stationarise the

following action-like quantity

$$\int dt \langle \Psi, t | i\partial_t - H | \Psi, t \rangle \equiv \int dt d\mathbf{x} \Psi^*(\mathbf{x}, t) (i\partial_t - H) \Psi(\mathbf{x}, t) \quad (1.23)$$

with the constraint $\langle \Psi, t | \Psi, t \rangle = 1$ which leads to the time-dependent Schrödinger equation.

In [31] it was shown that we can get a variational definition for the effective action $\Gamma[\bar{\varphi}]$, the generating functional of 1-particle-irreducible (1PI) diagrams, by minimising

$$\int dt \langle \Psi_-, t | i\partial_t - H | \Psi_+, t \rangle \quad (1.24)$$

where the states $\langle \Psi_-, t |$ and $|\Psi_+, t\rangle$ are constrained so that the matrix element of the fixed time Schrödinger picture operator $\hat{\phi}(\mathbf{x})$ is given by

$$\begin{aligned} \langle \Psi_-, t | \hat{\phi}(\mathbf{x}) | \Psi_+, t \rangle &= \bar{\varphi}(t, \mathbf{x}), \\ \langle \Psi_-, t | \Psi_+, t \rangle &= 1 \end{aligned} \quad (1.25)$$

and also the boundary condition these states tend to the ground state of H as $t \rightarrow \pm\infty$.

The physical theory is recovered when we remove the constraints by solving

$$\frac{\delta\Gamma[\bar{\varphi}]}{\delta\bar{\varphi}(\mathbf{x}, t)} = 0 \quad (1.26)$$

The effective action can also be defined as the Legendre transform of the functional generator of connected Green's functions $W[J]$,

$$\Gamma[\bar{\varphi}] = W[J] - \int dx \bar{\varphi}(x) J(x)$$

where $\bar{\varphi}(x) \equiv \delta W[J] / \delta J(x)$ (J is the source term) and $\delta\Gamma[\bar{\varphi}] / \delta\bar{\varphi}(x) = -J(x)$. As a consequence, the physical solutions which require vanishing of J , correspond to the stationary points of Γ and also to the removal of the constraints. Moreover, $\bar{\varphi}(x)$ is also the vacuum expectation value of the quantum field $\hat{\phi}$ in the presence of a source J ,

$$\bar{\varphi}(x) = \langle 0 | \hat{\phi}(x) | 0 \rangle_J$$

$$\bar{\varphi}_0(x) \equiv \bar{\varphi}(x)_{J=0}$$

so

$$\left. \frac{\delta\Gamma[\bar{\varphi}]}{\delta\bar{\varphi}(\mathbf{x}, t)} \right|_{\bar{\varphi}(x)=\bar{\varphi}_0(x)} = 0 \rightarrow \bar{\varphi}_0(x) = \langle 0 | \hat{\phi}(x) | 0 \rangle$$

The effective potential ⁵ V_{eff} is derived from the effective action assuming a constant background $\bar{\varphi}(x) = const$, i.e. $\bar{\varphi}(x)$ is independent of the space time point (translation invariance),

$$V_{eff}[\bar{\varphi}] \int dx \equiv -\Gamma[\bar{\varphi}] \Big|_{\bar{\varphi}=const} \quad (1.27)$$

where the infinite volume factor comes from the space time integrations.

Dirac's variational principle can then be used to obtain approximations by restricting the variation of the trial wave functional Ψ to the subspace of Gaussian trial states. In the following, we will explicitly write \hbar factors.

The most general Gaussian state can be written [31]

$$\begin{aligned} \Psi_t[\varphi] = N(t) \exp \left(- \int_{\mathbf{x}\mathbf{y}} (\varphi(\mathbf{x}) - \bar{\varphi}(\mathbf{x}, t)) \Omega(\mathbf{x}, \mathbf{y}, t) (\varphi(\mathbf{y}) - \bar{\varphi}(\mathbf{y}, t)) \right. \\ \left. + \frac{i}{\hbar} \bar{\pi}(\mathbf{x}, t) (\varphi(\mathbf{x}) - \bar{\varphi}(\mathbf{x}, t)) \right) \end{aligned} \quad (1.28)$$

where $N(t)$ is a normalisation constant and the integration in space $\int d^3\mathbf{x}$ was abbreviated as $\int_{\mathbf{x}}$. It will be convenient to separate the variational function Ω into real and imaginary parts [31]:

$$\Omega = \frac{1}{4\hbar} G^{-1}(\mathbf{x}, \mathbf{y}, t) - \frac{i}{\hbar} \Sigma(\mathbf{x}, \mathbf{y}, t). \quad (1.29)$$

Then variational parameters are $\bar{\varphi}$, $\bar{\pi}$, G and Σ . The physical meaning of the parameters of this wave functional is brought out by the following averages, considering $\langle \Psi | \Psi \rangle = 1$:

$$\begin{aligned} \langle \Psi | \hat{\phi}(\mathbf{x}) | \Psi \rangle &= \bar{\varphi}(\mathbf{x}, t) \\ \langle \Psi | \hat{\pi}(\mathbf{x}) | \Psi \rangle &= \bar{\pi}(\mathbf{x}, t) \end{aligned} \quad (1.30)$$

whereas the average value of the operator $i(\partial/\partial t)$ gives

$$\langle \Psi | i \frac{\partial}{\partial t} | \Psi \rangle = \int_{\mathbf{x}} \bar{\pi}(\mathbf{x}, t) \dot{\bar{\varphi}}(\mathbf{x}, t) + \int_{\mathbf{x}\mathbf{y}} \Sigma(\mathbf{x}, \mathbf{y}, t) \dot{G}(\mathbf{y}, \mathbf{x}, t) \quad (1.31)$$

showing that the imaginary part of the covariance function Ω plays the role of canonical conjugate momentum to the real part [8].

Now let us study the ϕ^4 theory given by the Hamiltonian (1.4) with $U(\phi) = \frac{m^2\phi^2}{2} + \frac{g}{4!}\phi^4$ within the context of the variational approximation for the Gaussian trial state. Substituting 1.28 into the Dirac's variational principle leads to

$$\Gamma[\bar{\varphi}, \bar{\pi}, G, \Sigma] = \int dt \langle \Psi | i \partial_t - H | \Psi \rangle = \int dt \int_{\mathbf{x}} \left(\left[\bar{\pi} \dot{\bar{\varphi}} - \frac{\bar{\pi}^2}{2} - \frac{(\nabla \bar{\varphi})^2}{2} - U(\bar{\varphi}) \right] \right)$$

⁵Also called generating functional of 1-PI Green's functions at zero energy and momentum.

$$\begin{aligned}
& +\hbar\left[(\Sigma\dot{G})(\mathbf{x},\mathbf{x},t) - 2(\Sigma G\Sigma)(\mathbf{x},\mathbf{x},t) - \left(\frac{1}{8}G^{-1}(\mathbf{x},\mathbf{x},t) - \frac{1}{2}\nabla_{\mathbf{x}}^2 G(\mathbf{x},\mathbf{y},t)\right)_{\mathbf{x}=\mathbf{y}} \right. \\
& \left. + \frac{1}{2}U^{(2)}(\bar{\varphi})G(\mathbf{x},\mathbf{x},t)\right] - \frac{\hbar^2}{8}G(\mathbf{x},\mathbf{x},t)G(\mathbf{x},\mathbf{x},t)U^{(4)}(\bar{\varphi}) \quad (1.32)
\end{aligned}$$

where $V(\bar{\varphi})$ denotes the classical potential, $U^{(n)}(\bar{\varphi}) = \frac{d^n U}{d\bar{\varphi}^n}$ and we used the matrix notation $(AB)(\mathbf{x},\mathbf{y}) = \int_{\mathbf{z}} A(\mathbf{x},\mathbf{z})B(\mathbf{z},\mathbf{y})$. We immediately recognise the the $O(\hbar^0)$ term as being the classical action. The variational equations with respect to the variational parameters $\delta\Gamma/\delta\bar{\varphi} = 0$, $\delta\Gamma/\delta\bar{\pi} = 0$, $\delta\Gamma/\delta\Sigma = 0$ and $\delta\Gamma/\delta G = 0$ give, respectively, the following set of equations [8],[27]

$$\begin{aligned}
\bar{\pi}(\mathbf{x},t) &= \dot{\bar{\varphi}}(\mathbf{x},t) \\
\dot{\bar{\pi}}(\mathbf{x},t) &= \left(\nabla_{\mathbf{x}}^2 \bar{\varphi} - U^{(1)}(\bar{\varphi}) - \frac{1}{2}U^{(3)}(\bar{\varphi})G(\mathbf{x},\mathbf{x},t)\right) \\
\dot{G}(\mathbf{x},\mathbf{y},t) &= 2\left((G\Sigma)(\mathbf{x},\mathbf{y},t) + (\Sigma G)(\mathbf{x},\mathbf{y},t)\right) \\
\dot{\Sigma}(\mathbf{x},\mathbf{y},t) &= \frac{1}{8}G^{-2}(\mathbf{x},\mathbf{y},t) - 2\Sigma^2(\mathbf{x},\mathbf{y},t) - \frac{1}{2}\left(-\nabla_{\mathbf{x}}^2 + U^{(2)}(\bar{\varphi})\right) \\
& \quad + \frac{\hbar}{2}U^{(4)}(\bar{\varphi})G(\mathbf{x},\mathbf{x},t)\delta^3(\mathbf{x}-\mathbf{y}). \quad (1.33)
\end{aligned}$$

This equations can be used to determine the vacuum of ϕ^4 -theory in this approximation [59],[27]. For this purpose, we assume translation invariance, which implies that $\bar{\varphi}$ is homogeneous and consequently the kernels can be expressed as a fourier transform

$$G(\mathbf{x},\mathbf{y}) = \int \frac{d^3\mathbf{p}}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})} \tilde{G}(\mathbf{p}) \quad (1.34)$$

considering that, for the vacuum functional, the kernels are time-independent. Therefore (1.33) results $\bar{\pi} = \Sigma = 0$ and

$$\begin{aligned}
\tilde{G}(\mathbf{p}) &= \frac{1}{2\sqrt{\mathbf{p}^2 + M^2}} \\
M^2 &= m^2 + \frac{g}{2}\bar{\varphi}^2 + \frac{g}{2} \int \frac{d^3\mathbf{p}}{(2\pi)^3} \tilde{G}(\mathbf{p}). \quad (1.35)
\end{aligned}$$

Notice that when $g = 0$, it reduces to the free vacuum functional (1.18). Since (1.35) is self-consistent for M^2 ⁶, it retains some of the non-linearities of the full quantum theory. Of course these statements are meaningful only upon renormalisation of the ultraviolet infinities. To illustrate this, we proceed to calculate the (renormalised) effective potential defined according to (1.27). Hence, for a homogeneous background, translation invariance implies $\dot{\bar{\varphi}} = 0 = \bar{\pi}$, $\dot{G} = 0 = \Sigma$, which with (1.32) and (1.33) enables us to write

$$V_{eff}(\bar{\varphi}) = \frac{1}{2}m^2\bar{\varphi}^2 + \frac{g}{4!}\bar{\varphi}^4 + \frac{\hbar}{4}G^{-1}(\mathbf{x},\mathbf{x}) + \frac{\hbar^2}{8}gG(\mathbf{x},\mathbf{x})G(\mathbf{x},\mathbf{x}), \quad (1.36)$$

⁶ M is usually called effective mass.

where G satisfies the equation

$$\frac{1}{4}G^{-2}(\mathbf{x}, \mathbf{y}) = (-\nabla^2 + m^2 + \frac{g}{2}\bar{\varphi}^2 + \hbar\frac{g}{2}G(\mathbf{x}, \mathbf{x}))\delta^3(\mathbf{x} - \mathbf{y}). \quad (1.37)$$

which using (1.34) determines G to be just (1.35). Hence the effective potential can be rewritten as [27]

$$\begin{aligned} V_{eff}(\bar{\varphi}) &= \frac{1}{2}m^2\bar{\varphi}^2 + \frac{g}{4!}\bar{\varphi}^4 - \frac{1}{2g}(M^2 - m^2 - \frac{g}{2}\bar{\varphi}^2)^2 \\ &+ \frac{M^2}{2}I_1 - \frac{M^4}{2}I_2(\Lambda) + \frac{M^4}{64\pi^2}(\ln\frac{M^2}{\Lambda^2} - \frac{1}{2}) \quad \text{where} \\ I_1 &= \int \frac{d^3p}{(2\pi)^3} \frac{1}{2|\mathbf{p}|} \quad \text{and} \\ I_2 &= \frac{1}{\Lambda^2} \int \frac{d^3p}{(2\pi)^3} \left(\frac{1}{2|\mathbf{p}|} - \frac{1}{2\sqrt{\mathbf{p}^2 + \Lambda^2}} \right) \quad (\Lambda \text{ is a mass scale}). \end{aligned} \quad (1.38)$$

The effective mass written in terms of I_1 and I_2 becomes

$$M^2 = m^2 + \frac{g}{2}I_1 + \frac{g}{2}\bar{\varphi}^2 - \frac{g}{2}M^2I_2 + \frac{g}{32\pi^2}M^2\ln\frac{M^2}{\Lambda^2}. \quad (1.39)$$

The theory possesses two divergent quantities I_1 and I_2 so we need to renormalise it. This can be achieved by redefining its two independent parameters namely the mass and the coupling constant (m and g). The effective potential becomes finite using the following renormalisation prescription ⁷

$$\begin{aligned} \left. \frac{dV_{eff}}{dM^2} \right|_{\Lambda_0} &= \frac{m_R^2}{g_R} \\ \left. \frac{d^2V_{eff}}{d(M^2)^2} \right|_{\Lambda_0} &= \frac{1}{3g_R} \end{aligned} \quad (1.40)$$

which can be rewritten with V_{eff} from (1.38) and (1.39) as

$$\begin{aligned} \frac{m_R^2}{g_R} &= \frac{m^2}{g} + \frac{1}{2}I_1 \\ \frac{1}{g_R} &= \frac{1}{g} + \frac{1}{2}I_2. \end{aligned} \quad (1.41)$$

Hence,

$$V_{eff} = -\frac{M^4}{2g_R} + \frac{M^2}{2}\bar{\varphi}^2 + \frac{m_R^2}{g_R}M^2 + \frac{M^4}{64\pi^2} \left[\ln\frac{M^2}{\Lambda^2} - \frac{1}{2} \right] \quad (1.42)$$

and the effective mass

$$M^2 = m_R^2 + \frac{g_R}{2}\bar{\varphi}^2 + \frac{g_R}{32\pi^2}M^2\ln\frac{M^2}{\Lambda^2} \quad (1.43)$$

⁷This is the same renormalisation prescription that has been used in the large- N approximation for this model [35]

The result above reflects some nonlinearities of the theory and can be used, for instance, to study its symmetry breaking mechanism. However, in quantum field theory the Gaussian approximation is far from reproducing the accuracy which is achieved when applied to quantum mechanical problems, as it was insightfully discussed by Feynman in [20]. The results which can be derived in this approximation are qualitatively equivalent to the large- N expansion and suffer from the same shortcomings. For example, while in quantum mechanics the energy level of the atoms could be predicted with great accuracy within the variational method using Gaussian states, in quantum field theory, although it is reasonably effective to determine the existence of bound states, it leads to a vanishing binding energy [27].

1.4 Fermionic Fields

The coordinate representation of fermionic operators presents some peculiarities owing to their anticommuting character. This leads us to introduce anticommuting functions in analogy with the Grassman numbers. In other words, we deal with the infinite-dimensional limit of the Grassman algebra $\{\eta, \eta\} = 0$, $\{d/d\eta, \eta\} = 1$, $\{d/d\eta, d/d\eta\} = 0$, $\int d\eta \equiv 0$ and $\int d\eta \eta \equiv 1$. We shall briefly discuss its main features in this section, following the original work on the functional representation for fermionic quantum fields by Floreanini and Jackiw [30].

A spin 1/2 field theory can be described by the Lagrangian

$$\mathcal{L} = \frac{i}{2} \psi \alpha^\mu \partial_\mu \psi - U(\psi) = \frac{i}{2} \psi \dot{\psi} - \mathcal{H}(\psi) \frac{i}{2} \quad (1.44)$$

with $\alpha^0 = \hat{1}$, $\{\alpha^i, \alpha^j\} = 2\delta^{ij}$ and ψ is a hermitian field satisfying the (equal time) anticommutation relations

$$\{\psi_a(\mathbf{x}), \psi_b(\mathbf{x}')\} \Big|_{x_0=x'_0} = \delta_{ab} \delta^3(\mathbf{x} - \mathbf{x}'). \quad (1.45)$$

Let us illustrate the problem of finding a functional representation for the quantum fermion field in its most elementary setting. Consider a massless Weyl-Majorana field in two space-time dimensions. It is described by a hermitian ($\psi^\dagger = \psi$), one component spinor field for which the anticommutation relations above simplify to $\{\psi(x), \psi(y)\} = \delta(x - y)$. We can consider our functional space as consisting of functionals $\Psi[u]$ of a Grassman field $u(x)$ such that at fixed time $\{u(x), u(y)\} = 0$ and each functional is associated with a ket,

$|\Psi\rangle \leftrightarrow \Psi[u]$. The question is how to define the action of the operator $\hat{\psi}(x)$ on this space. Since the field operators are their own momentum conjugates, they cannot be represented by their eigenvalues as we did for the scalar field. Instead we try a linear combination of their eigenvalues and the functional differential operators with respect to them, viz.

$$\psi(x)|\Psi\rangle = \left(\alpha u(x) + \beta \frac{\delta}{\delta u(x)} \right) \Psi[u] \quad (1.46)$$

The equal time commutation relations require that $\alpha\beta = 1/2$ and hence we choose $\alpha = \beta = 1/\sqrt{2}$. The Grassmanian character of the fields require careful treatment for the inner products. In order to gain some intuition, let us follow Jackiw [30] and consider the problem on a space $\{x\}$ consisting of two points $i = 1, 2$ on which two fermion operators are defined, satisfying $\{\psi(i), \psi(j)\} = \delta_{ij}$. A state $|\Psi_f\rangle$ is represented by a functional of $u(i)$ that can be expanded in a four dimensional basis

$$\Psi_f[u] = f_0 + f_1 u(1) + f_2 u(2) + f_{12} u(1)u(2) \quad (1.47)$$

The inner product with another state $|\Psi_g\rangle$ defined in a natural way as

$$\langle \Psi_g | \Psi_f \rangle = g_0^* f_0 + g_1^* f_1 + g_2^* f_2 + g_{12}^* f_{12} = \langle \Psi_f | \Psi_g \rangle^* \quad (1.48)$$

can be expressed as

$$\langle \Psi_g | \Psi_f \rangle = \int d^2 u \Psi_g^*[u] \Psi_f[u] \quad (1.49)$$

if

$$\langle \Psi_g | \rightarrow \Psi_g^*[u] = g_{12}^* + g_2^* u(1) - g_1^* u(2) + g_0^* u(1)u(2) \quad (1.50)$$

because only the Grassmanian integral $\int d^2 u u(1)u(2) = 1$ is non-vanishing. In fact, since the Grassman delta function is given by $\delta^2(u - \tilde{u}) = (u(1) - \tilde{u}(1))(u(2) - \tilde{u}(2))$, $\int d^2 \tilde{u} \delta^2(u - \tilde{u}) \Psi[\tilde{u}] = \Psi[u]$, (1.50) can be written as

$$\Psi_g^*[u] = \left(g_0^* - \sum_i g_i^* \frac{\delta}{\delta u(i)} + \frac{1}{2} \sum_{ij} g_{ij}^* \frac{\delta^2}{\delta u(j) \delta u(i)} \right) \delta^2(u). \quad (1.51)$$

Thus the adjoint of $u(i)$ is $\delta/\delta u(i)$ and $1/\sqrt{2}(u(i) + \delta/\delta u(i))$ is hermitian as it should be. The dualisation can be formulated analytically by introducing the auxiliary variables $\bar{u}(i)$ and an auxiliary dual functional $\bar{\Psi}_g[\bar{u}]$ defined by the natural formula

$$\bar{\Psi}_g[\bar{u}] = g_0^* + g_1^* \bar{u}(1) + g_2^* \bar{u}(2) + g_{12}^* \bar{u}(2) \bar{u}(1). \quad (1.52)$$

Therefore (1.50) can be written as ⁸

$$\Psi_g^*[u] = \int d^2\bar{u} e^{(\bar{u}(1)u(1) + \bar{u}(2)u(2))} \bar{\Psi}_g[\bar{u}] \quad (1.53)$$

with $\int d^2\bar{u} \bar{u}(2)\bar{u}(1) = 1$ being the only non-vanishing integral. The generalisation to field theory is immediate. Given $\Psi[u]$, construct $\bar{\Psi}[\bar{u}]$ by complex conjugating scalars and replacing $u(x)$ by $\bar{u}(x)$. Then the dual of $\Psi[u]$ is

$$\Psi^*[u] = \int \mathcal{D}\bar{u} e^{\int dx \bar{u}(x)u(x)} \bar{\Psi}[\bar{u}]. \quad (1.54)$$

1.5 Gauge Field Theories

In spite of being a bosonic theory, gauge field theories present some peculiar characteristics because of the gauge degrees of freedom. It turns out that the Schrödinger representation is particularly good to deal with them as we illustrate in this section.

Firstly let us set up our conventions. The vector potential A_μ may be presented as an element of the gauge's group Lie's algebra,

$$A_\mu = gA_\mu^a T_a \quad (1.55)$$

$T_a^\dagger = -T_a$, $[T_a, T_b] = f_{abc}T_c$, $\text{tr}T_a T_b = -\frac{1}{2}\delta_{ab}$ where the group indices run from 1 to the dimension of the group ($N^2 - 1$, for $SU(N)$) and the Lagrangian density reads

$$\mathcal{L} \equiv -\frac{1}{4}F^{\mu\nu a} F_{\mu\nu a} = \frac{1}{2g^2} \text{tr} F^{\mu\nu} F_{\mu\nu} \quad (1.56)$$

$$\begin{aligned} F_{\mu\nu}^a &= \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g f_{abc} A_\mu^b A_\nu^c \\ F_{\mu\nu} &= g F_{\mu\nu}^a T_a = \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu] \end{aligned} \quad (1.57)$$

The theory is invariant under local gauge transformations effected by an element U of the gauge group:

$$A_\mu \rightarrow A_\mu^U \equiv U^{-1} A_\mu U + U^{-1} \partial_\mu U, \quad (1.58)$$

$$F_{\mu\nu} \rightarrow F_{\mu\nu}^U \equiv U^{-1} F_{\mu\nu} U. \quad (1.59)$$

The Euler-Lagrange equations follow by varying A_μ in (1.56)

$$\partial_\mu F^{\mu\nu} + [A_\mu, F^{\mu\nu}] \equiv D_\mu F^{\mu\nu} = 0, \quad (1.60)$$

⁸Also known as Berezin integral.

and $F_{\mu\nu}$ satisfies the Bianchi Identity

$$D_\alpha F_{\beta\gamma} + D_\beta F_{\gamma\alpha} + D_\gamma F_{\alpha\beta} = 0 \quad (1.61)$$

The Hamiltonian formulation of Yang Mills theory is usually done in the temporal (or Weyl) gauge in which the temporal component of the gauge potential is set to zero. This is convenient in the canonical formalism since the momentum conjugate to A_0 vanishes. The canonical variables are the gauge potentials A_a^i and their conjugate momenta

$$\pi_a^i = \frac{\delta \mathcal{L}}{\delta \partial_0 A_a^i} = F_a^{0i} = \partial_0 A_a^i. \quad (1.62)$$

The Hamiltonian coincides with the energy (the zero-zero component of the stress energy tensor θ^{00}) and can be written as

$$H = \int d^3\mathbf{x} \mathcal{H} = \frac{1}{2} \int d^3\mathbf{x} \text{tr}(\mathbf{E}^2 + \mathbf{B}^2) \quad (1.63)$$

where

$$\begin{aligned} \mathcal{H} &= \pi_a^i \partial_0 A_a^i - \mathcal{L}, \\ E_a^i &\equiv F_a^{i0} = -\pi_a^i = -\dot{A}_a^i \quad \text{and} \\ B_a^k &= -\frac{1}{2} \epsilon^{kij} F_{ij}^a. \end{aligned} \quad (1.64)$$

The (equal time) canonical commutation relations

$$[E_a^i(\mathbf{x}, t), A_b^j(\mathbf{x}', t)] = i \delta_{ab} \delta^{ij} \delta^3(\mathbf{x} - \mathbf{x}') \quad (1.65)$$

leads naturally to a functional differential representation for the colour electric field, namely

$$E_a^i(\mathbf{x}) = i \frac{\delta}{\delta A_a^i(\mathbf{x})}, \quad (1.66)$$

acting on functionals of A_a^i . Since $A_0 = 0$, the Gauss Law (the time component of the Yang-Mills equation of motion) cannot be obtained neither by varying the Lagrangian, nor as a Hamiltonian equation. We can see from (1.60) that its time component is a fixed time constraint between canonical variables, namely

$$G_a \equiv (\mathbf{D} \cdot \mathbf{E})_a = 0 \quad (1.67)$$

Therefore the Gauss Law has to be imposed as a constraint on the physical states of the theory and will result in an additional functional differential equation which, in addition

to the Schrödinger equation, has to be satisfied by the wave functionals $\Psi[\mathbf{A}]$. It turns out that the Gauss law constraint implies that the wave functionals representing the physical states are gauge invariant. To see this, we start by recognising that the theory in the Weyl gauge has a residual symmetry under time independent local gauge transformations $U = e^{\theta^a(\mathbf{x})T^a}$, under which the gauge choice $A_a^0 = 0$ is preserved, whose infinitesimal form $U = 1 + \theta^a(\mathbf{x})T^a$ is

$$\delta A_a^i = -\frac{1}{g}(D^i\theta)_a \quad (1.68)$$

which is generated by $G \equiv D^i E_i$ and is conserved as it can be read off from the commutators:

$$\begin{aligned} i\left[H, \int d^3\mathbf{x} \theta^a(\mathbf{x})G_a(\mathbf{x})\right] &= 0, \\ i\left[\int \theta^b(\mathbf{y})G_b(\mathbf{y}), A_a^i(\mathbf{x})\right] &= \delta A_a^i(\mathbf{x}). \end{aligned} \quad (1.69)$$

Moreover, it satisfies an algebra that follows from the group Lie algebra:

$$i[G_a(\mathbf{x}), G_b(\mathbf{y})] = gf_{abc}G_c(\mathbf{x})\delta(\mathbf{x} - \mathbf{y}) \quad (1.70)$$

The above is a very important relation. It enables us to impose the condition on the physical states

$$G|\Psi\rangle_{phys} = 0 \quad (1.71)$$

The problem is that (1.71) actually represents an infinite number of equations, one for each spatial point \mathbf{x} since G is also the generator of a local symmetry. Hence questions concerning integrability, for instance, arise. Such questions can be answered by analysing the commutator of two constraints since, as G generates the symmetry transformation, one expects their commutator to follow the Lie algebra (1.70). If this relation holds, the constraints are consistent (technically called first class) and the constraint equations are integrable, at least locally [29]. Generically speaking, anomalous terms could appear owing to the infinities of a local quantum field theory (ultraviolet divergencies), and in many cases they are essential to render the quantum theory meaningful as it is the case of the (quantum) symmetry breaking of undesirable symmetries present at classical level [33]⁹.

⁹For example, for the anomalous chiral Schwinger Model, an equivalent equation to (1.70) holds with Poisson brackets at classical level but acquires a quantum extension (anomaly) at quantum level, obstructing the Gauss' law. However, the suitably constructed quantum theory which removes this obstruction leads to the expected massive excitations in this model [36]

In view of (1.70), (1.71) translates into a functional differential equation for the physical wave functionals

$$\left(\partial_i \frac{\delta}{\delta A_a^i(\mathbf{x})} - gf_{abc} A_b^i(\mathbf{x}) \frac{\delta}{\delta A_c^i(\mathbf{x})} \right) \Psi[\mathbf{A}] = 0 \quad (1.72)$$

which amounts to say that $\Psi[\mathbf{A}]$ is invariant under spatial gauge transformations. To see this, recall that a change in the wave functional by a variation in its argument reads

$$\delta\Psi[\mathbf{A}] = \int d^3\mathbf{x} \frac{\delta\Psi[\mathbf{A}]}{\delta A_a^i(\mathbf{x})} \delta A_a^i(\mathbf{x}) \quad (1.73)$$

Using (1.68), we get $\delta A_a^i = -\frac{1}{g}(\partial^i\theta_a + gf_{abc}A_b^i\theta_c)$ which taken into the equation above, after an integration by parts gives

$$\delta\Psi[\mathbf{A}] = \int d^3\mathbf{x} \theta_a \left(\partial_i \frac{\delta}{\delta A_a^i(\mathbf{x})} - gf_{abc} A_b^i(\mathbf{x}) \frac{\delta}{\delta A_c^i(\mathbf{x})} \right) \Psi[\mathbf{A}] \quad (1.74)$$

which for $\theta_a \neq 0$ implies (1.72).

A class of finite gauge transformations is obtained by exponentiating the generator of infinitesimal transformations $F \equiv -\frac{1}{g} \int d^3\mathbf{x} \theta^a(\mathbf{x}) G_a(\mathbf{x})$ [34], namely e^{iF} . Therefore, the invariance of the physical states under the finite transformations which are formed by iterating the infinitesimal version is expressed by

$$e^{iF} |\Psi\rangle = |\Psi\rangle \quad (1.75)$$

or in terms of the wave functional

$$e^{iF} \Psi[\mathbf{A}] = \Psi[\mathbf{A}'] \quad (1.76)$$

where \mathbf{A}' is the gauge transformation of \mathbf{A} . This applies only to those finite gauge transformations which are obtained by iterating (exponentiating) the infinitesimal one. For this class of transformations U is deformable to the identity. They are referred to as “small gauge transformations”. It remains to verify what happens to a broader class of gauge transformations, i.e. those which are not formed by iterating an infinitesimal one (so called large gauge transformations). This issue is related to a vast topic in gauge field theory, concerning its topological properties. Here we restrict ourselves to show how some concepts can be more easily understood within the functional Hamiltonian formalism, particularly the θ angle in $(3+1)$ -dimensional gauge theories.

1.5.1 θ -angle in Yang-Mills Theory

We start our discussion with Yang-Mills theories in the 3-dimensional space time. One can add to the Lagrangian a Chern-Simons term. This term gives mass to the vector fields yet the equation of motion is gauge covariant. The Lagrangian density is

$$\mathcal{L} = \frac{1}{2g^2} \text{tr} F^{\mu\nu} F_{\mu\nu} - \frac{\tilde{\mu}}{2g^2} \epsilon^{\mu\nu\alpha} \text{tr} (F_{\mu\nu} A_\alpha - \frac{2}{3} A_\mu A_\nu A_\alpha), \quad (1.77)$$

where $\tilde{\mu}$ has the dimension of mass and $\tilde{\mu}/g^2$ is dimensionless¹⁰. This mass term is believed to carry a topological significance which is seen from studying quantisation. There is also a beautiful connection with Yang Mills theories in 4 space-time dimensions (considered at high temperatures)[32]. Roughly speaking, because of the periodic boundary conditions imposed on the fields, finite temperature field theory in the imaginary time formalism lives in $\mathbb{R}^3 \times S^1$ and the radius of S^1 is given by $1/T$. In the limit when $T \rightarrow \infty$, S^1 collapses leaving a three dimensional space \mathbb{R}^3 ¹¹. With this in mind, there are grounds to make a connection between the four dimensional structures responsible for the θ vacua and those leading to the mass term in three dimensions, thus lending support to the conjecture that the latter arises from the former in a high temperature reduction.

Consider a finite gauge transformation (1.58) in (1.77). The action changes by

$$\int d^3x \mathcal{L} \rightarrow \int d^3x \mathcal{L} + \frac{\tilde{\mu}}{g^2} \int d^3x (\epsilon^{\alpha\beta\mu} \partial_\alpha \text{tr} [\partial_\beta U U^{-1} A_\mu]) + \frac{8\pi^2 \tilde{\mu}}{g^2} w(U), \quad (1.78)$$

where

$$w(U) = \frac{1}{24\pi^2} \int d^3x \epsilon^{\alpha\beta\gamma} \text{tr} [\partial_\alpha U U^{-1} \partial_\beta U U^{-1} \partial_\gamma U U^{-1}] \quad (1.79)$$

If we restrict the gauge transformations that tend to the identity at the spatial and temporal infinity $\lim_{x \rightarrow \infty} U(x) = \pm \mathbf{I}$ ¹² the A -dependent surface integral above vanishes. The other term can also be transformed into a surface integral once the integrand is rewritten as a total derivative. As a matter of illustration we introduce a explicit parametrisation for U and choose $SU(2)$ as the gauge group:

$$\begin{aligned} U(x) &= e^{T^\alpha \theta_\alpha(x)} \\ T^\alpha &= \frac{\sigma^\alpha}{2i}, \quad \theta_\alpha = \hat{\theta}^\alpha |\theta|. \end{aligned} \quad (1.80)$$

¹⁰The fact that the mass term is a world scalar (independent of the metric) is an evidence for its topological nature.

¹¹Plus a dimensionful rescaling of the coupling constant $g \rightarrow Tg$

¹²This restriction is made in order to avoid convergence problems in (1.78) and also reflects an assumption of space time uniformity. See [28] for a complete discussion.

Therefore $w(U)$ is written as

$$w(U) = \int d^3x \partial_\alpha \tilde{w}^\alpha = -\frac{1}{16\pi^2} \int d^3x \epsilon^{\alpha\beta\gamma} \epsilon^{abc} \partial_\alpha [\hat{\theta}^a \partial_\beta \hat{\theta}^b \partial_\gamma \hat{\theta}^c (|\theta| - \sin|\theta|)] \quad (1.81)$$

which although being a surface integral, can be shown to take integer values which characterise the so-called homotopy class to which U belongs. Only for the homotopically trivial class (that in which U can be continuously deformed to the identity), $w(U)$ does vanish¹³.

Let us analyse the consequences of this results to the quantised version of the theory. We have seen that the action (1.78) is not gauge invariant and changes by

$$\tilde{\mu} \times (8\pi^2) \times w(U) = \tilde{\mu} \times (8\pi^2) \times \text{integer} . \quad (1.82)$$

However, in the quantum theory it is the exponential of the action that should be gauge invariant, that is $\exp(i \int d^3x \mathcal{L})$. Therefore a change in the action makes a consistent quantum theory only if it is an integral multiple of 2π and we are led to the quantisation condition

$$4\pi \frac{\tilde{\mu}}{g^2} = n \quad (n, \text{integer}) \quad (1.83)$$

The Euclidean formulation leads to the same conclusion [32]. We can also give a Hamiltonian derivation of the quantisation rule, based on the response of the system to (spatial) two-dimensional gauge transformations. It turns out that (1.83) is a consequence of the Gauss' law as a necessary condition for its global integrability. In contrast to the four dimensional Yang-Mills theory, in three space-time dimensions static gauge transformations have zero winding number [28], in other words, there is only one homotopy class for the two-dimensional gauge function U . They are all "small" and can be implemented by exponentiating the infinitesimal generator¹⁴. The Euler Lagrange equations which follow from (1.77) are

$$D_\mu F^{\mu\nu} + \frac{\tilde{\mu}}{g^2} \frac{\epsilon^{\nu\alpha\beta} F_{\alpha\beta}}{2} = 0 \quad (1.84)$$

¹³A little of mathematical terminology will be useful in what follows. The gauge functions U with large distance asymptotes $\pm I$ provide a mapping of the 3-sphere S^3 , which is equivalent to the three space R^3 once the points at infinite are identified, into the gauge group. Such mappings fall into disjoint homotopy classes labeled by integers, and gauge functions belonging to different classes cannot be continuously deformed in one another. Particularly only those which belong to the zero class are deformable to the identity. For example, consider a mapping $S^3 \rightarrow SU(2)$. Since the three parameters that specify this group also form a S^3 space, we have $S^3 \rightarrow S^3$, mathematically expressed as $\Pi^3(SU(2)) = \Pi^3(S^3) = \mathcal{Z}$ (group of integers under addition). It is also true that $\Pi^n(S^n) = \mathcal{Z}$ and $\Pi^n(S^m) = 0$, for $n < m$, meaning that all mappings can be deformed into a single mapping (i.e. the topology is trivial) [66]

¹⁴Physically this means that there is no θ -angle in two spatial dimensions and mathematically that $\Pi^2(S^m) = 0$, $m > 2$

Because of the mass term, the canonically conjugated momentum acquires an extension, namely $\pi_a^i = -E_a^i + \tilde{\mu}/(2g^2)\epsilon^{ij}A_a^j$ in the Weyl gauge. A modified form of the Gauss' law, has to be imposed in the physical states, as the time component of (1.84)

$$(\mathbf{D}\cdot\mathbf{E})_a + \frac{\tilde{\mu}}{g^2} \frac{\epsilon^{ij}F_{ij}^a}{2} = 0 \quad (1.85)$$

has an extension. In canonical variables, this equation writes as

$$G_a \equiv -(D_i \pi^i)_a + \frac{\tilde{\mu}}{g^2} \frac{\epsilon^{ij} \partial_i A_j^a}{2}.$$

It can be shown that this G_a commutes with the Hamiltonian and satisfies the Lie algebra (1.70), which guarantees the local integrability of the Gauss's law. $G_a|\Psi\rangle = 0$ translates into

$$\left(D_i \frac{\delta}{\delta A_a^i} \right) \Psi[\mathbf{A}] - i \frac{\tilde{\mu}}{g^2} \frac{\epsilon^{ij} \partial_i A_j^a}{2} \Psi[\mathbf{A}] = 0, \quad (1.86)$$

or upon iteration

$$e^{-\frac{i}{g} \int d^2 \mathbf{x} \theta^a G_a} \Psi[\mathbf{A}] = \Psi[\mathbf{A}]. \quad (1.87)$$

The left hand side of (1.87) can be written as

$$e^{-\frac{i}{g} \int d^2 \mathbf{x} \theta^a G_a} \Psi[\mathbf{A}] = e^{i \frac{8\pi^2 \tilde{\mu} \Omega(\theta)}{g^2}} \Psi[\mathbf{A}^U] \rightarrow \Psi[\mathbf{A}^U] = e^{-i \frac{8\pi^2 \tilde{\mu} \Omega(\theta)}{g^2}} \Psi[\mathbf{A}] \quad (1.88)$$

$$\Omega(\theta) \equiv \frac{1}{8\pi^2} \int d^2 \mathbf{x} \epsilon^{ij} \text{tr}(\partial_i U U^{-1} A^j) - \int d^2 \mathbf{x} \tilde{w}^0 \quad (1.89)$$

where \tilde{w}^0 , is the time component of \tilde{w}^α defined as in (1.81)¹⁵. As we know from quantum mechanics that whenever a symmetry transformation on a canonical variable changes the Lagrangian by a total time derivative of a function, that function appears as a phase in the transformation law for the quantum mechanical state. Therefore, in our case,

$$L \rightarrow L - \frac{d}{dt} \left(\frac{8\pi^2 \tilde{\mu}}{g^2} \Omega(\theta) \right) \quad (1.90)$$

Finally, the quantisation of the mass comes as follows: Although the Gauss's law is locally integrable as it is guaranteed by the commutators of G_a , we will have to examine its global integrability. Mathematically speaking, the statement that Π^3 is non-trivial implies that the space of gauge functions U defined on the two space is not simply connected [66]. Now consider a 3-dimensional U which is not deformable to the identity. We can view U is a family of two dimensional matrices depending on the spatial two vector \mathbf{x} and a parameter τ such that as $\tau \rightarrow \pm\infty$, $U \rightarrow \mathbf{I}$ [34]. In other words, we have a loop that starts and ends

¹⁵For $SU(2)$ it would be $-1/(16\pi^2) \int d^2 \mathbf{x} \epsilon^{ij} \epsilon^{abc} \hat{\theta}^a \partial_i \hat{\theta}^b \partial_j \hat{\theta}^c (|\theta| - \sin|\theta|)$.

at the identity yet it cannot be deformed to the identity by hypothesis. If we follow (1.88) as τ varies from $-\infty$ to $+\infty$, with $U = \mathbf{I}$ at the endpoints, the phase factor must be unity¹⁶, or equivalently

$$\frac{8\pi^2\tilde{\mu}}{g^2}\Omega(\theta)\Big|_{-\infty}^{\infty} = \frac{8\pi^2\tilde{\mu}}{g^2} \int_{-\infty}^{\infty} d\tau \frac{\partial}{\partial\tau}\Omega(\theta) = 2\pi n \quad (1.91)$$

The integral in the expression above can be identified with $w(U)$ which is itself an integer. Therefore we arrive again at the quantisation condition (1.83) as a constraint so that the Gauss' law is globally integrable.

Let us turn our attention to the four space time dimensional case. For small gauge transformations (those for which U is deformable to the identity, the physical content of (1.76) is that the wave functionals are gauge invariant:

$$\Psi[\mathbf{A}'] = \Psi[\mathbf{A}]. \quad (1.92)$$

However, for gauge transformations which cannot be deformed to the identity or, if you like, that cannot be composed by iterating an infinitesimal gauge transformation, one cannot assert that the wave functional remains invariant when these “large” gauge transformations are performed. Let us call \mathcal{G}_n the operator which implements a gauge transformation in the n^{th} homotopy class to which U belongs. Thus, we say that only \mathcal{G}_0 has the representation e^{iF} . \mathcal{G}_n is unitary and commutes with the Hamiltonian, since it generates a symmetry transformation. From general quantum mechanical principles, we conclude that the physical states are eigenvectors of \mathcal{G}_n , with an eigenvalue which is a pure phase:

$$\mathcal{G}_n\Psi[\mathbf{A}] = \Psi[\mathbf{A}'] = e^{-i\theta_n}\Psi[\mathbf{A}]. \quad (1.93)$$

Owing to the additive nature of the gauge function's homotopic characterisation, it is clear that $\theta_n = n\theta$.

This is the origin of the θ angle, which appears naturally in a Hamiltonian formulation of the theory. It is possible to remove the phase from the transformation law above, provided we find a functional of \mathbf{A} , which we call $w(\mathbf{A})$, that changes by n when a gauge transformation in the n^{th} homotopy class is performed, i.e.

$$w(\mathbf{A}') = w(\mathbf{A}) + n. \quad (1.94)$$

¹⁶The first term in (1.89) vanishes when $U = \mathbf{I}$.

We start out by writing

$$\Psi[\mathbf{A}] = e^{-i\theta w(\mathbf{A})} \Phi[\mathbf{A}] \quad (1.95)$$

where $\Phi[\mathbf{A}]$ is invariant against all gauge transformations

$$\mathcal{G}_n \Phi[\mathbf{A}] = \Phi[\mathbf{A}'] = \Phi[\mathbf{A}]. \quad (1.96)$$

Such functional can indeed be constructed and it is

$$w(\mathbf{A}) = \frac{-1}{16\pi^2} \int d^3\mathbf{x} \epsilon^{ijk} \text{tr}[F_{ij} A_k - \frac{2}{3} A_i A_j A_k]. \quad (1.97)$$

We have already seen that gauge transformations change $w(\mathbf{A})$ according to (1.78). There, $w(U)$ labels U homotopy classes and is an integer number. Now, a universal phase factor can be removed from all the wave functionals at the cost of adding a total time derivative to the Lagrangian. If the quantum theory based on the functionals Ψ is obtained from a Lagrangian $L_\Psi = \int d^3\mathbf{x} \mathcal{L}$, the one based on the functionals $\Phi = e^{-i\theta w(\mathbf{A})} \Psi$ is obtained from the Lagrangian

$$L_\Phi = \int d^3\mathbf{x} \mathcal{L} + \theta \frac{dw(\mathbf{A})}{dt}. \quad (1.98)$$

We can be shown that

$$\frac{dw(\mathbf{A})}{dt} = \frac{-1}{16\pi^2} \int d^3\mathbf{x} \text{tr} *F^{\mu\nu} F_{\mu\nu} \quad (1.99)$$

where $*F^{\mu\nu} = \frac{1}{2} \epsilon^{\mu\nu\alpha\beta} F_{\alpha\beta}$ is the dual strength tensor. This enables us to define a new Lagrangian

$$\mathcal{L} = -\frac{1}{4} F_a^{\mu\nu} F_{\mu\nu}^a + \frac{g^2}{32\pi^2} \theta *F_a^{\mu\nu} F_{\mu\nu}^a, \quad (1.100)$$

and since the second term is a total divergence,

$$\begin{aligned} *F_a^{\mu\nu} F_{\mu\nu}^a &= \partial_\mu X^\mu \\ X^\mu &= \epsilon^{\mu\alpha\beta\gamma} \text{tr}[F_{\alpha\beta} A_\gamma - \frac{2}{3} A_\alpha A_\beta A_\gamma], \end{aligned} \quad (1.101)$$

it does not change the equations of motion. $w(A) = -\frac{g^2}{4\pi^2} \int d^3\mathbf{x} X^0$, is exactly the winding number defined before. In summary, the θ -angle in Yang-Mills theories is present even by imposing gauge invariance on the wave functionals¹⁷. If we recall that the theory in 3 space-time dimensions is the high temperature limit of the theory in 4, and that the coupling rescales like $g \rightarrow gT$ we see that the quantisation condition for the mass term of the three dimensional theory leads to

$$\mu = \frac{g^2}{4\pi} n \propto nT \quad (1.102)$$

¹⁷The θ term in the Lagrangian is CP odd and thus it could be a source of CP -violation in nature.

and therefore we can say that a non vanishing mass term (3-dimensional space time) presumably arises from a non vanishing θ (4-dimensional space time) and the discontinuities in the former for the three dimensional model are suggestive of different phases in the latter.

1.5.2 BRST Symmetry in the Schrödinger Representation

When we quantise a gauge field theory, for instance in the path integral formalism, we have spurious infinities which reflect the integration over equivalent gauge configurations. A way out this problem is the Faddeev-Popov functional integral procedure which is basically a selection of one representative from every set of gauge equivalent potentials (orbit) [55]. This is done by a modification in the integration measure which, exponentiated, amounts to additional terms in the Lagrangian which includes anticommuting scalar fields called “ghosts”. Despite the gauge invariance of this (effective) Lagrangian being broken by gauge fixing terms and the Faddeev-Popov ghosts, it is still invariant under a well known class of transformations of the fields called Becchi-Rouet-Stora Transformations (*BRST*).

The Schrödinger representation is particularly good in dealing with gauge degrees of freedom and in understanding the relation between quantisation procedures between different gauge-fixing conditions [67]. In [39], it was shown that the *BRST* quantisation of gauge field theories could be carried out solely within the Schrödinger picture. They showed that *BRST* symmetry can be considered as the residual gauge symmetry of the gauge fixed Lagrangian and hence the correct form of the Hamiltonian/Lagrangian comes out naturally from this formalism. This interpretation has given a new insight in understanding the origin of the *BRST* symmetry as well as provided a new method of obtaining the *BRST* structure of a theory [40]. Let us illustrate these arguments in their simplest setting.

For simplicity, consider the abelian gauge theory Lagrangian density:

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu}. \quad (1.103)$$

Let us adopt the covariant gauge for which the gauge potential satisfies the gauge-fixing condition

$$\partial_\mu A^\mu - a(x) = 0, \quad (1.104)$$

where $a(x)$ is an arbitrary scalar function. The gauge fixing condition can be translated into the insertion of Lagrangian multipliers, namely

$$\bar{\mathcal{L}} = \mathcal{L} + \pi_0 \partial_\mu A^\mu + \frac{1}{2} \alpha \pi_0^2, \quad (1.105)$$

where α is a gauge parameter, and treating all the variables in the equation above on equal footing (independent). Nevertheless, $\bar{\mathcal{L}}$ is still invariant under $A^\mu \rightarrow A^\mu + i\partial^\mu \chi$ where χ satisfies $\partial_\mu \partial^\mu \chi = 0$. This residual degree of freedom should not affect any physical information. This condition translates into the wave functional formalism as

$$\Psi_{phys}[A^\mu(\mathbf{x}) + i\partial^\mu \chi(\mathbf{x}, t), t] = \Psi_{phys}[A^\mu(\mathbf{x}), t]. \quad (1.106)$$

Now, we write $\chi(\mathbf{x}, t) = \lambda \eta(\mathbf{x}, t)$, where λ is an infinitesimal Grassman number and η a Grassman variable. The condition (1.106) written in terms of these variables reads:

$$\int d^3\mathbf{x} \partial^\mu \eta(\mathbf{x}, t) \frac{\delta}{\delta A^\mu(\mathbf{x})} \Psi_{phys}[A^\mu(\mathbf{x}), t] = 0, \quad (1.107)$$

with $\eta(\mathbf{x}, t)$ satisfying the equation $\partial_\mu \partial^\mu \eta(\mathbf{x}, t) = 0$ which is considered as an additional variable to those in $\bar{\mathcal{L}}$. This equation can also be written as

$$\begin{aligned} \bar{\mathcal{P}} &= -i\dot{\eta}, \\ \dot{\bar{\mathcal{P}}} + i\nabla^2 \eta &= 0. \end{aligned} \quad (1.108)$$

The equation of motion for η can be included as part of the Euler Lagrange equations by writing the Lagrangian as

$$\mathcal{L}_{new} = \bar{\mathcal{L}} - \mathcal{P}(\dot{\eta} - i\bar{\mathcal{P}}) - \bar{\eta}(\dot{\bar{\mathcal{P}}} + i\nabla^2 \eta), \quad (1.109)$$

which is the correct form of the Lagrangian including the gauge fixing and ghost terms. From the equation above, we obtain the Hamiltonian

$$H = \int d^3\mathbf{x} [\mathcal{H}_{gauge} - \frac{1}{2} \alpha \pi_0^2 - \pi_0^2 \nabla \cdot \mathbf{A} - i\mathcal{P}\bar{\mathcal{P}} - i\nabla\bar{\eta} \cdot \nabla\eta]. \quad (1.110)$$

The (anti)commutation relations

$$\begin{aligned} [\pi_\mu(\mathbf{x}), A_\nu(\mathbf{x}')] &= -i g_{\mu\nu} \delta^3(\mathbf{x} - \mathbf{x}'), \\ \{\eta(\mathbf{x}), \mathcal{P}(\mathbf{x}')\} &= -i \delta^3(\mathbf{x} - \mathbf{x}'), \\ \{\bar{\eta}(\mathbf{x}), \bar{\mathcal{P}}(\mathbf{x}')\} &= -i \delta^3(\mathbf{x} - \mathbf{x}'), \end{aligned} \quad (1.111)$$

render functional derivatives as representatives for the operators, $\pi_\mu(\mathbf{x}) = i\delta/\delta A^\mu(\mathbf{x})$, $\mathcal{P}(\mathbf{x}) = -i\delta/\delta\eta(\mathbf{x})$, $\bar{\mathcal{P}}(\mathbf{x}) = -i\delta/\delta\bar{\eta}(\mathbf{x})$, which allow us to write (1.107) as

$$\Omega\Psi_{phys}[A^\mu, t] = 0,$$

$$\Omega = \int d^3\mathbf{x} [-i\bar{\mathcal{P}}\pi_0 + \eta\nabla\cdot\mathbf{E}],$$

and we immediately recognise the operator Ω as the *BRS* charge operator, and the condition above is nothing but the *BRS* condition over the physical states [68]¹⁸. The same can be done for the non-abelian theory.

1.5.3 Abelian Gauge Theory Vacuum Functional

The ground state wave functional for the photon field theory is exactly solvable. In (3+1)-dimensions, adopting the temporal gauge, the Hamiltonian is written

$$H = \frac{1}{2} \int d^3\mathbf{x} (\mathbf{E}^2 + \mathbf{B}^2), \quad (1.112)$$

where $E_i(\mathbf{x}) = -\dot{A}_i(\mathbf{x})$, $\mathbf{B}(\mathbf{x}) = \nabla \wedge \mathbf{A}(\mathbf{x})$. In the coordinate Schrödinger representation, where the operator $\hat{A}_i(x)$ is diagonal, $\hat{E}_i(\mathbf{x}) = i\delta/\delta A_i(\mathbf{x})$ is the differential representation of the equal-time commutators. Hence we obtain the following form for eigenvalue problem:

$$\frac{1}{2} \int d^3\mathbf{x} \left(-\frac{\delta}{\delta A(\mathbf{x})} \cdot \frac{\delta}{\delta A(\mathbf{x})} + \mathbf{B}(\mathbf{x})\cdot\mathbf{B}(\mathbf{x}) \right) \Psi[\mathbf{A}] = E\Psi[\mathbf{A}]. \quad (1.113)$$

The Gauss' law constraint on the physical states is simpler than in the non-abelian case. It is written as

$$\partial_i \frac{\delta}{\delta A_i(\mathbf{x})} \Psi[\mathbf{A}] = 0 \quad (1.114)$$

and its physical content can immediately be brought out. The change in the wave functional due to a abelian gauge transformation for which $\delta A_i = -\partial_i\theta$ can be calculated as

$$\begin{aligned} \delta\Psi[\mathbf{A}] &= - \int d^3\mathbf{x} \frac{\delta\Psi[\mathbf{A}]}{\delta A_i(\mathbf{x})} \partial_i\theta \\ &= \int d^3\mathbf{x} \nabla \cdot \frac{\delta\Psi[\mathbf{A}]}{\delta \mathbf{A}} \theta(\mathbf{x}) \end{aligned} \quad (1.115)$$

¹⁸The anticommuting character of the variable η which was introduced to realise the degrees of freedom is important to assure the commutation of the operator Ω with the Hamiltonian. If one have chosen a tensor variable, Ω would not commute with H and hence it would be impossible to realise the residual symmetry transformations.

where in the last step we integrated by parts. It is obvious that the Gauss' law implies gauge invariance and that $\Psi[\mathbf{A}]$ depends only on the transverse components of \mathbf{A} . In other words, only $\Psi[\mathbf{A}_T]$ is gauge invariant (physical).

The Hamiltonian can be rewritten as

$$\begin{aligned} H_{EM} &= \frac{1}{2} \int d^3\mathbf{x} \left(-\frac{\delta}{\delta\mathbf{A}(\mathbf{x})} \cdot \frac{\delta}{\delta\mathbf{A}(\mathbf{x})} + A^i(\mathbf{x})h_{ij}A^j(\mathbf{x}) \right) \\ h_{ij} &\equiv -\nabla^2\delta_{ij} + \partial_i\partial_j, \end{aligned} \quad (1.116)$$

from which we clearly see it is quadratic and therefore it is simply the Hamiltonian of the infinite dimensional harmonic oscillator. Since we are looking for the ground state, we try a wave functional with no nodes and positive everywhere $\Psi_0[\mathbf{A}] = \mathcal{N}e^{-W[\mathbf{A}]}$ (\mathcal{N} is a normalisation constant). The Schrödinger equation becomes

$$\frac{1}{2} \int d^3\mathbf{x} \left(\frac{\delta^2 W}{\delta\mathbf{A}^2(\mathbf{x})} - \left(\frac{\delta W}{\delta\mathbf{A}(\mathbf{x})} \right)^2 + A^l(\mathbf{x})h_{lm}A^m(\mathbf{x}) \right) = E_0 \quad (1.117)$$

On dimensional counting basis, we claim that W is quadratic in A , resulting in a Gaussian wave functional for the vacuum

$$W = \frac{1}{2} \int d^3\mathbf{x} d^3\mathbf{y} A^i(\mathbf{x})w_{ij}(\mathbf{x},\mathbf{y})A^j(\mathbf{y}). \quad (1.118)$$

If we take (1.118) back into the Schrödinger equation we get

$$\int d^3\mathbf{z} w_{ik}(\mathbf{x},\mathbf{z})w_{kj}(\mathbf{z},\mathbf{y}) = h_{lm}\delta^3(\mathbf{x}-\mathbf{y}) \quad (1.119)$$

which we solve by using the Fourier transform method to obtain

$$w_{ij}(\mathbf{x},\mathbf{y}) = (-\nabla^2\delta_{ij} + \partial_i\partial_j) \int \frac{d^3\mathbf{p}}{(2\pi)^3} \frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{|\mathbf{p}|}. \quad (1.120)$$

Finally, the vacuum functional can be written as

$$\begin{aligned} \Psi_0[\mathbf{A}] &= \mathcal{N} \exp\left(-\frac{1}{(2\pi)^2} \int d^3\mathbf{x} d^3\mathbf{y} \frac{\mathbf{B}(\mathbf{x})\cdot\mathbf{B}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2} \right) \\ &= \mathcal{N} \exp\left(-\frac{1}{8\pi^2} \int d^3\mathbf{x} d^3\mathbf{y} \frac{F_{ij}(\mathbf{x})F_{ij}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2} \right), \end{aligned} \quad (1.121)$$

which is explicitly gauge invariant. The excited states can be constructed by acting with functional representation of the creation operator on (1.121) as we did for the scalar fields.

1.5.4 Yang-Mills Vacuum Functional (YMFV)

As we pointed out in the introduction, the biggest difficulty in analysing the strong interaction resides in its large distance behaviour where perturbation theory cannot be applied.

In this sense, phenomena like confinement, and the bound state spectrum are poorly understood. All these problems concern the ground state of a non-abelian gauge theory whose physical understanding is of major importance. In this sense, as far as analytical approaches are concerned, the SRQFT has become a good framework to deal with these problems, at least within the standard model¹⁹, although we still lack a complete analysis of the matter owing to some difficulties which have motivated our work.

The difficulty in applying, for example, a variational ansatz to solve the Schrödinger equation for the ground state of a non-abelian gauge theory starts with the fact that it is impossible to write down a Gaussian wave functional which satisfies the constraint of gauge invariance as can be easily verified. The Gaussian wave functional

$$\Psi[\mathbf{A}] = e^{-\frac{1}{2} \int d^3x d^3y [A_i^a(x) - \zeta_i^a(x)] (G^{-1})_{ij}^{ab}(x,y) [A_j^b(y) - \zeta_j^b(y)]} \quad (1.122)$$

transforms under gauge transformations (1.58) as $\Psi(\mathbf{A}) \rightarrow \Psi(\mathbf{A}^U)$. In the Abelian case, it is sufficient to take $\partial_i G_{ij}^{-1} = 0$ to satisfy the Gauss' law constraint (1.72). However, in the non-abelian case, due to the homogeneous piece in (1.58), no gauge invariant Gaussian wave functional exists²⁰. Following Feynman [20], another obstacle that arises is what he called the "sensitivity of the variational procedure to high frequencies". In contrast to abelian gauge theories, Yang-Mills theories are non-linear and consequently the high and low momentum modes are coupled. On the other hand, the vacuum expectation value of the energy and other intensive quantities is dominated by high momentum fluctuations (there are infinitely more ultraviolet modes than modes with low momentum). So, for example, in the search for information involving low momentum modes, even if we have a good approximation for the wave functional in this region, if the ultraviolet part is slightly incorrect the minimisation of the energy may have nothing to do with the dynamics of the low momentum modes themselves. Moreover, physical information beyond the Gaussian trial faces the problem of calculability of the resulting functional integrals.

A lot of physics would emerge from the solution of the non-abelian analogue of equation (1.113) (see (1.62) - (1.66)),

$$\frac{1}{2} \int d^3\mathbf{x} d^3\mathbf{y} \left(- \frac{\delta}{\delta \mathbf{A}^a(\mathbf{x})} \cdot \mathbf{K}^{ab}(\mathbf{x}, \mathbf{y}; \epsilon) \cdot \frac{\delta}{\delta \mathbf{A}^b(\mathbf{y})} + \frac{1}{2} (F_{ij}^a)^2 \right) \Psi[\mathbf{A}] = E \Psi[\mathbf{A}] \quad (1.123)$$

¹⁹There has been some progress in understanding non-perturbative aspects in the context of supersymmetric gauge theory [76]

²⁰Some attempts have been made to remedy this problem, for instance projecting the Gaussian wave functional onto the gauge invariant sector [13].

subjected to the Gauss' law constraint that the wave functionals are gauge invariant. \mathbf{K} regularises the product of two functional derivatives at the same (spatial) point, which is ill-defined²¹. Unfortunately, it is much easier to formulate this equation than to solve it.

Notwithstanding, approximate forms of the YMVF have been constructed for particular configurations of the fields. They have been useful to verify confinement and give some estimates for the mass of the glueballs. The latter are bound states formed by strong self interaction of gluons. Bag Models, Instanton Gas Models and Lattice simulations place the lightest glueball mass in the range $1.5 \rightarrow 1.8 GeV$ ²² [75],[62](for a review, see [70]).

It is believed that the low hadron spectrum originates mainly from long-wavelength excitations, that is field configurations for which $\mathbf{A}(\mathbf{x})$ varies slowly in comparison with the confinement scale [61]. This is also the large distance or strong-coupling limit, in an infrared enslaving theory. In this limit, it was firstly suggested by Greensite that the YMVF has the form [46]

$$\Psi_0[\mathbf{A}] = \exp\left(-\mu \int d^3\mathbf{x} \text{tr} (F_{ij}(\mathbf{x}))^2\right) \quad (1.124)$$

where F_{ij} is the magnetic component of the colour field strength. Notice that the probability density Ψ_0^2 looks like e^{-S} with S being the Euclidean classical action in one dimension lower (dimensional reduction). A lattice version of (1.124) was obtained in a strong coupling expansion for the gauge group $SU(2)$ in $(2+1)$ dimensions [43] and in $(3+1)$ dimensions [44]. It was verified that $\mu(\beta)$, where β is the conventional coupling that enters the Wilson action ($\beta \propto 1/g^2$), behaves like $constant \times \beta$, in the strong coupling region and scales correctly in the continuum limit (weak coupling) as required by the renormalisability of the theory.

A continuum strong coupling expansion of the YMVF was derived by Mansfield [1] and gives (1.124) as the leading order ground state with $\mu = \gamma/g^2$ and γ a constant which depends on the number of colours.

It is instructive to compare (1.124) with the abelian wave functional (1.121). It includes a factor $\Delta(\mathbf{x} - \mathbf{y}) = 1/|\mathbf{x} - \mathbf{y}|^2$ which reflects that the system has an infinite correlation length, i.e. it is conformally invariant. Clearly (1.124) is not the correct vacuum functional for all scales. Because of asymptotic freedom, we expect that the true vacuum resembles

²¹It obviously has the property $\lim_{\epsilon \rightarrow 0} \mathbf{K}^{ab}(\mathbf{x}, \mathbf{y}; \epsilon) = \delta(\mathbf{x} - \mathbf{y})\delta^{ab} \mathbf{1}$.

²²The mass of the proton is $\approx 0.94 GeV$

(1.121) at short distances. Rather (1.124) is the effective vacuum functional in the strong coupling limit.

A simple interpolating form which contains the two limiting cases, namely short and large wave-length configurations, was proposed by Arisue in [41]. In $(3 + 1)$ -dimensions it writes:

$$\Psi_0[\mathbf{A}] = \exp\left(-\int d^3\mathbf{x}d^3\mathbf{y} \operatorname{tr} [F_{ij}(\mathbf{x})V(\mathbf{x}, \mathbf{y})F_{ij}(\mathbf{y})V(\mathbf{y}, \mathbf{x})] \frac{e^{-\xi^{-1}|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|^2}\right) \quad (1.125)$$

where is a Wilson line (a gauge connector between the points \mathbf{x} and \mathbf{y})²³ and ξ represents the correlation length for the field strength in the vacuum. If we take $F_{ij}(\mathbf{y})$ and $V(\mathbf{y}, \mathbf{x})$ and expand \mathbf{y} around \mathbf{x} , after an integration over \mathbf{y} , we arrive at [41]

$$\Psi_0[\mathbf{A}] = \exp\left(-\mu_0 \int d^3\mathbf{x} \operatorname{tr}(F_{ij})^2 - \mu_2 \int d^3\mathbf{x} \operatorname{tr}(D_i F_{ij})^2 + \dots\right) \quad (1.126)$$

in which the dots stand for higher covariant derivative terms. We see from (1.126) that for sufficiently low momenta and small amplitudes (i.e, a slowly varying field configuration) the covariant derivative can be neglected and (1.124) recovered. He also used a Monte Carlo simulation of $SU(2)$ in $(2 + 1)$ dimensions to calculate the expansion coefficients $\mu_0 = (0.91 \pm 0.02)/g^2$ and $\mu_2 = -(0.19 \pm 0.05)/g^6$, where g is the renormalised coupling constant. The correlation length, which is related to the mass gap, is written in terms of these coefficients as $\xi = \sqrt{(-2\mu_2)/\mu_0}$.

In [1] it was shown that (1.124) leads to confinement (the Wilson loop satisfies an area law [74]) via a kind of dimensional reduction from $(3 + 1)$ to $(1 + 1)$ dimensions. Yang-Mills theory in 2 dimensions is manifestly “infrared slaving” even in perturbation theory because the Coulomb potential in 2 dimensions increases linearly for large distance separations [71]. Greensite in [20], based on the concept of magnetic disorder which establishes that confinement is associated with disorder in the field strength F_{ij} , argues that (1.124) is the wave functional with maximum possible disorder in F_{ij} for small amplitude fluctuations. Despite the success in describing confinement, in order to calculate the glueball spectrum we would have to include more rapidly varying fields in 1.126 as we will discuss in section 2.2.

²³ $V(\mathbf{x}, \mathbf{y}) = \mathcal{P} \exp(i \int_{\mathbf{x}}^{\mathbf{y}} \mathbf{A}(\mathbf{x}') \cdot d\mathbf{x}')$.

1.6 Renormalisable Theories in the Schrödinger Representation

It was relatively recently that the question of renormalisability of quantum field theory in the Schrödinger representation was studied from a more rigorous and formal standpoint [5]. This is partially because isolating and renormalising divergences in quantum field theory is effected more conveniently in the Lorentz covariant Green's function formalism. As the language of wave functionals started to provide significant contributions to field theoretic problems, the issue of their renormalisability became crucial.

When Symanzik set off to solve this problem, he was initially motivated by a special two-dimensional case, namely the relativistic string model in which the Schrödinger wave functionals are the primary objects of physical interest [52] and the problem of the ultraviolet finiteness of the Casimir force in renormalisable quantum field theories which would follow from a mathematically well defined proof of the existence of its Schrödinger representation.

Here we briefly discuss some ideas contained in [5] which will be important in the next chapters. We suggest [6] for an introduction to [5].

As we discussed in the first sections, in the Schrödinger representation we work with wave functionals of a time-independent, c-number field $\varphi(\mathbf{x})$ (see equations (1.5)-(1.13))²⁴, namely $\Psi[\varphi]$. Its interpretation is that $|\Psi[\varphi]|^2$ is proportional to the probability for the quantum field $\hat{\phi}(x)$ to assume the value $\varphi(\mathbf{x})$ at the time t , (our space-like quantisation hypersurface) which we conventionally choose to be $t = 0$. In other words the operator $\hat{\phi}(\mathbf{x}, 0)$ is diagonal in the Schrödinger representation, viz.

$$\hat{\phi}(\mathbf{x}, 0)\Psi[\varphi] = \varphi(\mathbf{x})\Psi[\varphi] \quad (1.127)$$

and choosing the equal time commutation relations between the operator $\hat{\phi}$ and its canonically conjugated momentum $\hat{\pi}$ also at $t = 0$ gives

$$\hat{\pi}(\mathbf{x}, 0)\Psi[\varphi] = -i\frac{\delta}{\delta\varphi(\mathbf{x})}\Psi[\varphi] \quad (1.128)$$

as a coordinate representation for the momentum. The dynamics of the system is governed by the time-dependent Schrödinger equation (1.12) in which the Hamiltonian is also defined

²⁴We will be talking about scalar fields but our arguments generalise to fermions and gauge fields.

on the hypersurface $t = 0$. Hence we can say that the Schrödinger equation is the relation that the wave functional has to satisfy upon (smooth local) deformations of the boundary $t = 0$, which is represented by time differentiation [9]. Then, after finding the solution $\Psi_t[\varphi]$, the boundary takes the form of a quantisation surface $t = 0$ from where the solution can be extended to the whole plane making use of the time evolution operator $e^{i\hat{H}t}$.

The wave functionals can also be represented as functional integrals, their argument being the boundary value of the field. To see that, consider the matrix element

$$\langle \varphi | e^{-TH} | \varphi' \rangle, \quad (1.129)$$

the Euclidean propagation kernel for going from a field configuration at Euclidean time $t = 0$ to another at Euclidean time $t = -T$, also known as Schrödinger functional. According to Feynman, this can be represented as

$$\int \mathcal{D}\phi e^{-S_E[\phi]} \quad (1.130)$$

in which the fields satisfy boundary conditions $\phi(\mathbf{x}, t = 0) = \varphi$ and $\phi(\mathbf{x}, t = -T) = \varphi'$ and S_E is the Euclidean action for the $D + 1$ -dimensional volume (where ϕ lives), bounded by space-like surfaces a time T apart. By inserting a complete set of eigenstates of the Hamiltonian H , $\{|E_n\rangle\}$ into the Schrödinger functional we arrive at its spectral representation. As $T \rightarrow \infty$, this is dominated by the contribution of the ground state,

$$\begin{aligned} \langle \varphi | e^{-TH} | \varphi' \rangle &= \sum_n \Psi_n[\varphi] \Psi_n^*[\varphi'] e^{-TE_n} \\ &\xrightarrow{T \rightarrow \infty} \Psi_0[\varphi] \Psi_0^*[\varphi'] e^{-TE_0}. \end{aligned}$$

Assuming that φ' vanishes at $T = \infty$ and normalised the vacuum energy such that $E_0 = 0$ enables us to write

$$\Psi_0[\varphi] = \int \mathcal{D}\phi e^{-S_E[\phi]} \quad (1.131)$$

with $\phi(t = 0) = \varphi$. In summary, the Schrödinger functional naturally leads to the concept of a quantum field theory on a manifold with boundaries.

Since perturbative renormalisability of quantum field theory is usually established using power counting in the momentum space, in the case of the Schrödinger functional this is no longer feasible as translation invariance is lost in the time direction. In other words we cannot rely on Lorentz invariance in our task to renormalise the theory. A priori,

it is not clear if a renormalisable quantum field theory in the compact space time manifold remains renormalisable in the presence of a boundary. We present below a summary of Symanzik's results regarding this matter and some of their implications for our work [5],[6],[7],[53].

- Symanzik studied the Schrödinger functional of ϕ^4 scalar field theory in perturbation theory in $(3 + 1)$ -dimensions. He found that the Schrödinger functional, and therefore the wave functional, is finite as any cut-off is removed provided that besides the usual renormalisation procedure for the divergences that occur in the bulk of the space-time, two new counterterms are introduced. These counterterms are needed because of additional divergences that result from the boundary conditions and are proportional to the local composite fields $\phi\partial_t\phi$ and ϕ^2 integrated over the hyperplanes at $t = 0$ and $t = -T$ ²⁵.
- These new divergences appear because the field operators which are diagonalisable in the sense of the Schrödinger representation differ from the usual renormalised field operators by (in perturbation theory, logarithmically) divergent factors, similarly as the renormalised field operators themselves differ by such factors from the "bare" field operators. That is to say, relation (1.127) does not hold, but there is a substitute

$$\lim_{t \rightarrow 0} a(t)\phi(x)\Psi[\varphi] = \varphi(\mathbf{x})\Psi[\varphi] \quad (1.132)$$

where $a(t)$ is a singular coefficient given to first order by

$$a(t) = 1 - g/(64\pi^2)[\ln(\mu^2 t^2) + \ln(4\pi) - \Gamma'(1) + 2] + O(g^2),$$

where μ is the normalisation mass in the minimal subtraction scheme of dimensional regularisation.

- Consequently, the argument of the vacuum functional (1.131), i.e the boundary values of the scalar field must be renormalised in a way that differs from the usual quantum field theory without boundaries. In (1.131) the boundary condition reads

$$\phi(\mathbf{x}, 0) = Z_s\varphi(\mathbf{x}) \quad (1.133)$$

where Z_s denotes a new renormalisation constant, which is needed to cancel the extra ultraviolet divergences introduced by the boundary at $t = 0$. Within the dimensional regularisation scheme, in $4 - \epsilon$ dimensions one finds $Z_s = 1 - (g/32\pi^2)1/\epsilon + O(g^2)$.

²⁵In dimensional regularisation only $\phi\partial_t\phi$ suffices.

- This is believed to be the case for a generic renormalisable quantum field theory: The wave functionals are finite as any cut-off is removed when they are constructed as functional integrals, after the inclusion of a finite number of additional boundary counterterms. These are local polynomials in the fields and their derivatives, integrated over the boundary. Furthermore they must respect the symmetries of the theory and have canonical dimension less than or equal to three in a $(3 + 1)$ -dimensional theory.
- In the case of Yang-Mills theory there are no local gauge invariant composite field of dimension three or less if invariance under parity is assumed. This was confirmed in $SU(N)$ Yang-Mills theory to one loop order in perturbation theory in [7]. In the language of the eigenvalue problem expressed by the Yang-Mills Schrödinger equation, this amounts to say that it is sufficient to regulate the divergences introduced by the laplacian and renormalise them in a way that both the wave functional and the eigenvalues are finite as any cut-off is removed.
- For QCD , Sint in [50] studied the Schrödinger functional to one loop order of perturbation theory. Using dimensional regularisation and heat kernel techniques to determine the divergences, he verified that they are partly canceled by the usual renormalisations of the quark mass and the coupling constant in QCD . An additional divergence could be absorbed in a multiplicative renormalisation of the quark boundary fields whose corresponding boundary counterterm is a local polynomial in the fields in agreement with Symanzik expectations.

Chapter 2

A Large Distance Expansion for the Vacuum Functional

For fields that vary slowly on the scale of the inverse of the mass of the lightest physical particle, the logarithm of the vacuum functional of a quantum field theory has a derivative expansion in terms of *local* functions. This is the basis of a scheme in which, by studying its analyticity properties under complex scalings, the vacuum functional can be reconstructed for arbitrary fields from its local expansion.

2.1 Introduction

As we discussed in the introductory chapter, whilst asymptotic freedom has led to an accurate determination of the Lagrangian of the standard model from high energy experiments, there are only a few analytical tools enabling us to calculate with that Lagrangian at low energies, where the semi-classical expansion is no longer valid. Therefore, the computation of the so called low-hadron spectrum, for example, can only be done numerically using lattice gauge field theory. Analytical studies may provide more physical insight into these problems and the interplay between analytical and numerical approaches can certainly assist either approach in obtaining new methods and results. In this and the following chapters we discuss an approach to quantum field theory in which states are constructed in the Schrödinger representation from their large distance behaviour as it was proposed by Mansfield in [2].

At large distances the logarithm of the vacuum functional, $\ln \Psi_0[\varphi] = \ln e^{W[\varphi]} = W[\varphi]$, undergoes a significant simplification for any theory in which the lightest physical mass

is non-zero. It can be expanded in a sum of local functionals in the sense that it can be reduced to a single spatial integral of a sum of terms each of which is constructed from the field and a finite number of its derivatives evaluated at the same spatial point.

In order to probe the internal structure of particles which are characterised by much shorter scales, such large distance expansion appears to be useless. However, it is one of the purposes of this chapter to show that this large distance expansion can be used to understand physics at all length scales since it may be used to reconstruct the vacuum functional, $\Psi[\varphi]$ say, for arbitrary $\varphi(\mathbf{x})$. This chapter is based on references [2] and [3].

2.2 Local nature of the vacuum functional at large distances

Let us firstly concentrate on scalar fields, for simplicity. In section (1.6) we showed how to build a functional integral representation for the vacuum functional $\Psi_0[\varphi]$, where φ was the boundary value of the field at $t = 0$. In what follows, it will be convenient to introduce a different formulation so to make the φ dependence more explicit, since it will appear in the functional integral. For this purpose, let us define a bra $\langle D|$, D for Dirichlet, which has the property of being annihilated by the field operator $\hat{\varphi}$,

$$\langle D|\hat{\varphi} = 0. \quad (2.1)$$

Thus we can represent $\langle\varphi|$ by

$$\langle\varphi| = \langle D| \exp\left(i \int d\mathbf{x} \hat{\pi}(\mathbf{x})\varphi(\mathbf{x})\right) \quad (2.2)$$

so that

$$\frac{\delta}{\delta\varphi(\mathbf{x})}\langle\varphi| = i\langle\varphi|\hat{\pi}(\mathbf{x}), \quad (2.3)$$

and using the canonical commutation relations and (2.1) we also recover $\langle\varphi|\hat{\varphi}(\mathbf{x}) = \varphi(\mathbf{x})\langle\varphi|$. Hence, we can write

$$\langle\varphi|e^{-T\hat{H}}|\varphi'\rangle = \langle D|e^{i \int d\mathbf{x} \hat{\pi}(\mathbf{x},0)\varphi(\mathbf{x})} e^{-T\hat{H}} e^{-i \int d\mathbf{x} \hat{\pi}(\mathbf{x},-T)\varphi'(\mathbf{x})}|D\rangle, \quad (2.4)$$

which in turn can be written as a functional integral ¹

¹Since $\hat{\pi} = \dot{\hat{\varphi}}$, $\hat{\pi}$ is represented in the functional integral by $\dot{\varphi}$ plus terms coming from the time derivative acting on the T -ordering because the functional integral represents T -ordered terms. This leads to terms like $\int dx_1 dx_2 \varphi(x_1)\varphi(x_2)\delta(x_1 - x_2)\delta(0) = \int \varphi^2(x)\delta(0)$. Because it is local, this additional term can be canceled by an opposite and equal counterterm in the functional integral which amounts to simply discarding this divergence. We will come back to this issue when we discuss the Feynman diagram expansion of the vacuum functional.

$$\int \mathcal{D}\phi \exp\{-S_E + \int d\mathbf{x} \dot{\phi}(\mathbf{x}, 0) \varphi(\mathbf{x}) - \int d\mathbf{x} \dot{\phi}(\mathbf{x}, -T) \varphi'(\mathbf{x})\} \quad (2.5)$$

and the variable ϕ defined on the Euclidean semi-plane $t \leq 0$ now satisfies boundary conditions $\phi(\mathbf{x}, 0) = \phi(\mathbf{x}, -T) = 0$ as it is implied by $\langle D \rangle$. Taking T to infinity where φ' is assumed to vanish, lead us to a functional integral representation of the vacuum functional on the Euclidean space-time $t \leq 0$:

$$\langle \varphi | E_0 \rangle \equiv \Psi_0[\varphi] = e^{W[\varphi]} = \int \mathcal{D}\phi \ e^{-S_E + \int d\mathbf{x} \dot{\phi}(\mathbf{x}) \varphi(\mathbf{x})} . \quad (2.6)$$

Hence, in a semi-classical expansion, $W[\varphi]$ is a sum of Euclidean connected Feynman diagrams in which φ is the source for $\dot{\phi}$ on the boundary where ϕ vanishes. They are obtained by contracting boundary values of the field with vertices using a propagator yielding a very non-local result. The only major difference from the usual Feynman diagrams in free space is that the propagator vanishes when either of its arguments lies on the boundary. Moreover, a formal proof that $W[\varphi]$ is a well defined quantity (is finite as any cut-off is removed) has been constructed by Symanzik [5] for φ_{3+1}^4 theory, as we discussed in section (1.6).

We can expand $W[\varphi]$ as

$$W[\varphi] = \sum_n \int d^D x_1 \dots d^D x_n \Gamma^{(n)}(x_1, \dots, x_n) \varphi(x_1) \dots \varphi(x_n) \quad (2.7)$$

which reflects its non-local character (here D is the space-time dimension). Now suppose that the lightest physical particle of the theory has a mass m . We want to study $W[\varphi]$ for fields that vary slowly in space on the scale of $1/m$. In other words let us choose to examine W when the Fourier transform of φ vanishes for momenta greater than the mass. If we expand the propagators used to contract the boundary fields as $1/(p^2 + m^2) = 1/m^2 - p^2/m^4 + (p^2)^2/m^6 + \dots$ which, in space time, gives an expansion in derivatives of delta functions

$$(-\partial^2 + m^2)^{-1} \delta^D(\mathbf{x} - \mathbf{x}') \delta(t - t') = \left(\frac{1}{m^2} - \frac{\partial^2}{m^4} + \frac{\partial^4}{m^6} - \dots \right) \delta^D(\mathbf{x} - \mathbf{x}') \delta(t - t') . \quad (2.8)$$

Using this, we are able to write a local expression for $W[\varphi]$ and since it is connected, it reduces to a single spatial integral of a sum of terms which are composed of powers of the field and a finite number of its derivatives calculated at the same point in contrast with a non-local expression which we would have if we evaluated it for more rapidly varying fields. Then (2.7) for slowly varying fields simplifies to

$$W[\varphi] = \int d^D \mathbf{x} \left(a_1 \varphi^2 + a_2 \varphi^4 + a_3 \varphi^6 \dots + b_1 \nabla \varphi \cdot \nabla \varphi + b_2 (\nabla \varphi \cdot \nabla \varphi)^2 + \dots + c_1 \varphi^2 \nabla \varphi \cdot \nabla \varphi \right)$$

$$+ c_2\varphi^2(\nabla\varphi\cdot\nabla\varphi)^2 + \dots + d_2\varphi^2\nabla^2\varphi\nabla^2\varphi + \dots + e_2\varphi^5\nabla^2\nabla^2\varphi + \dots \quad (2.9)$$

The coefficients of this expansion a_i, b_i , etc., are dimensionful constants which in principle can be determined by the Schrödinger equation which W satisfies. Also this local expansion has to obey the symmetries of the theory it describes. For example, in the local expansion we have written down only terms which are even under $\varphi \rightarrow -\varphi$ assuming that this is an unbroken symmetry of the action.

Let us give some specific examples of this simplification. Consider a free massive scalar field theory in $D+1$ dimensions. In the Schrödinger representation the Hamiltonian is (see (1.14))

$$H = -\frac{1}{2}\Delta + \int d^D\mathbf{x} \frac{1}{2} \left(\nabla\varphi \cdot \nabla\varphi + m^2\varphi^2 \right), \quad (2.10)$$

where Δ is the (unregulated) laplacian $\int d^D\mathbf{x} \frac{\delta^2}{\delta\varphi^2(\mathbf{x})}$. The vacuum functional has the form $e^W = \exp\{-\int \varphi G\varphi\}$ as we showed in (1.15), with G given by (1.16) and (1.17). Choosing $G = -\sqrt{-\nabla^2 + m^2}$ ensures that e^W is a normalisable eigenstate of the Hamiltonian with an eigenvalue E which is proportional to the functional trace of G . For a complex scalar field in a time-independent gauge potential background, we have only to replace ∇ with a covariant derivative. The simplification of the vacuum functional to a local expansion is achieved by expanding G as $-(m - \nabla^2/2m - (\nabla^2)^2/(8m^3) + \dots)$ to obtain

$$W_{local} \equiv \int d^D\mathbf{x} \left(\frac{m}{2}\varphi^2 + \frac{1}{4m}(\nabla\varphi)^2 - \frac{1}{16m^3}(\nabla^2\varphi)^2 + \dots \right) \quad (2.11)$$

which converges with the support that Fourier transform of φ lies within $p^2 < m^2$, that is, when the field varies slowly in space on the scale of the inverse of the mass. The same is true for an interacting theory in which the lightest particle has non-zero mass since massive propagators are exponentially damped at large distances. Hence, in configuration space, Feynman diagrams are small except when all their points are within a distance of $\approx 1/m$ of each other.

The Lagrangian density for a free massive Dirac field can be written in terms of two component Weyl spinors $\{\hat{u}, \hat{v}\}$ in the chiral representation as

$$\mathcal{L} = i(\hat{u}^\dagger \dot{\hat{u}} + \hat{v}^\dagger \dot{\hat{v}} - \hat{u}^\dagger \sigma \cdot \nabla \hat{u} + \hat{v}^\dagger \sigma \cdot \nabla \hat{v}) - m(\hat{u}^\dagger \hat{v} + \hat{v}^\dagger \hat{u}) \quad (2.12)$$

Choosing to diagonalise \hat{u} and \hat{v}^\dagger so that $\hat{u}|u, v^\dagger\rangle = u|u, v^\dagger\rangle$, $\hat{v}^\dagger|u, v^\dagger\rangle = v^\dagger|u, v^\dagger\rangle$ (u, v^\dagger are Grassman numbers) the canonical anti-commutation relations can be represented by

$\hat{u}^\dagger = \delta/\delta u$, $\hat{v} = \delta/\delta v^\dagger$ and the adjoint is with respect to a weighted inner product that yields the resolution of the identity as

$$1 = \int |u, v^\dagger\rangle \mathcal{D}(u^\dagger, u, v^\dagger, v) e^{\int d^3\mathbf{x}(uu^\dagger - vv^\dagger)} \langle u, v^\dagger|. \quad (2.13)$$

The Hamiltonian in this representation reads

$$H = \int d^3\mathbf{x} \left(-\frac{\delta}{\delta u} i\sigma \cdot \nabla u + v^\dagger i\sigma \cdot \nabla \frac{\delta}{\delta v^\dagger} + m \left(v^\dagger u + \frac{\delta}{\delta u} \frac{\delta}{\delta v^\dagger} \right) \right) \quad (2.14)$$

Assuming that the wave functional has the form $\Psi \equiv \langle u, v^\dagger | 0 \rangle = \exp \int d^3\mathbf{x} v^\dagger G_D u$, the Hamiltonian gives us

$$H\Psi = \left(\int d^3\mathbf{x} (v^\dagger \{G_D, i\sigma \cdot \nabla\} u + m(v^\dagger u - v^\dagger G_D G_D u)) + m \text{Tr}(G_D) \right) \Psi \quad (2.15)$$

which is $E\Psi$ with $E = m \text{Tr}(G_D)$ provided $\{G_D, i\sigma \cdot \nabla\} + m - m G_D G_D = 0$. This has the solution

$$G_D = i \frac{\sigma \cdot \nabla}{m} + \sqrt{1 - \frac{\nabla^2}{m^2}}. \quad (2.16)$$

Taking the minus sign corresponds to filling the Dirac sea so that all the other states have energy greater than the vacuum. The local form of the vacuum functional can be obtained by expanding G in powers of ∇^2/m^2 which will converge for slowly varying u, v^\dagger .

In pure Yang-Mills theory, there is no mass term in the Lagrangian. Notwithstanding, a non-zero glueball mass is expected to be generated quantum mechanically and therefore the full propagator of the gauge potential \mathbf{A} will again be expandable in powers of p^2/m^2 for small p^2 in comparison with the mass of the lightest glueball². In 3 + 1-dimensions, we would have

$$\begin{aligned} W[\mathbf{A}] \equiv \ln \Psi[\mathbf{A}] &= \int d^3\mathbf{x} (a_1 \text{tr} \mathbf{B} \cdot \mathbf{B} / \Lambda + a_2 \text{tr} D \wedge \mathbf{B} \cdot D \wedge \mathbf{B} / \Lambda^3 \\ &+ a_3 \text{tr} \mathbf{B} \cdot (\mathbf{B} \wedge \mathbf{B}) / \Lambda^3 + a_4 \text{tr} \mathbf{B} \cdot \mathbf{B} \mathbf{B} \cdot \mathbf{B} / \Lambda^5 + \dots) \end{aligned} \quad (2.17)$$

where we only included gauge and parity invariant terms. The unknown coefficients a_i are now dimensionless and assumed to be finite as the cut-off is removed. \mathbf{B} is the colour magnetic field $\nabla \wedge \mathbf{A} + \mathbf{A} \wedge \mathbf{A}$ and Λ is a renormalization group invariant mass. Since the mass depends non-perturbatively on the coupling constant, this expression will not result from working in a finite order in standard perturbation theory. The coefficients a_i are

²This is in contrast to the Abelian Gauge theory where W can be calculated exactly to give $W = -\frac{1}{4\pi^2 e^2} \int d^3\mathbf{x} d^3\mathbf{y} \mathbf{B}(\mathbf{x}) \cdot \mathbf{B}(\mathbf{y}) / (\mathbf{x} - \mathbf{y})^2$ which is conformally invariant and cannot be expanded in terms of local quantities.

in principle obtainable from a Yang-Mills-Schrödinger equation. This expansion is very useful to study large distances effects in which the dominant term is expected to be the one with the fewest number of derivatives, namely

$$\Psi[\mathbf{A}] \approx e^{a_1 \int d^3x \text{tr } \mathbf{B} \cdot \mathbf{B} / \Lambda} . \quad (2.18)$$

As we discussed in section (1.5.4), this term leads to an area law for the Wilson loop via a kind of dimensional reduction, and thus indicates that this approach is a good starting point for computation of low-energy processes in that theory. The first two terms in this expansion have been studied in lattice gauge field theory (see section (1.5.4)).

In order to get reliable results concerning, for instance, the low hadron spectrum, we will need to compute more terms in the local expansion of W . Although this local expansion has shown to be successful in describing large Wilson loops, it is only expected to converge for slowly varying fields on the scale of the lightest glueball mass. Thus it cannot be accurate for the computation of the glueball spectrum, for example, as this involves heavier particles and hence more rapidly varying fields. However, the analyticity properties of the vacuum functional under complex scalings provide an ingenious way to resum the local series so as to reconstruct the vacuum functional for arbitrary fields as we shall see.

2.3 Reconstructing the Vacuum Functional from its Large Distance Behaviour

We will start the discussion with an example. Let us return to the Hamiltonian of the free scalar field (2.10). We regulate the laplacian by introducing a momentum cut-off ϵ ,

$$\Delta_\epsilon = \int d^D x d^D y \int_{p^2 < \frac{1}{\epsilon}} \frac{d^D p}{(2\pi)^D} e^{ip(x-y)} \frac{\delta^2}{\delta\varphi(x)\delta\varphi(y)} = \int_{p^2 < \frac{1}{\epsilon}} d^D p (2\pi)^D \frac{\delta^2}{\delta\tilde{\varphi}(-p)\delta\tilde{\varphi}(p)} \quad (2.19)$$

where $\tilde{\varphi}(p) = \int d^D x \varphi(x) \exp -ip \cdot x$. The vacuum energy density $\mathcal{E} = E/V$ is now well-defined and diverges as the cut-off is removed

$$\mathcal{E} = \frac{1}{2V} \Delta_\epsilon W = \frac{1}{2} \int_{p^2 < \frac{1}{\epsilon}} \frac{d^D p}{(2\pi)^D} \sqrt{p^2 + m^2} \sim \frac{k}{(D+1)\epsilon^{(D+1)/2}} \quad \text{as } \epsilon \rightarrow 0 \quad (2.20)$$

where k is the area of the unit sphere in D dimensions divided by $2(2\pi)^D$. On the other hand if we apply the laplacian to our local expansion of W (2.11), we get

$$\frac{1}{2V} \Delta_\epsilon W_{local} = \int_{p^2 < \frac{1}{\epsilon}} \frac{d^D p}{(2\pi)^D} \left(\frac{m}{2} - \frac{p^2}{4m} - \frac{(p^2)^2}{16m^3} \dots \right) = \sum_{n=0}^{\infty} \frac{\alpha_n}{(m^2 \epsilon)^{n+D/2}} \quad (2.21)$$

(where $\alpha_n = km^{D+1}\Gamma(\frac{3}{2})/(\Gamma(3/2 - n)\Gamma(n + 1)(D + 2n))$). Notice that this expression appears to have divergencies of increasing order as $\epsilon \rightarrow 0$ unlike (2.20) which correctly gives the behaviour of the vacuum energy as the cut-off is removed. This is because the local expansion holds only for slowly varying fields, i.e. $\tilde{\varphi}(p)$ for which $p^2 < m^2$. Therefore the expression (2.21) only makes sense for $\epsilon m^2 > 1$, that is, large ϵ . In other words, the operation of removing the cut-off does not commute with expanding in local quantities even for the free theory. We can remedy this so as to use the large ϵ expansion in order to obtain the right one as it goes to zero by resumming the large ϵ -series. In order to agree with our future notation, let us scale $\epsilon \rightarrow \epsilon' = \epsilon s$. Now ϵ' plays the rôle of cut-off and we can set $\epsilon = 1$. Define the continuation of the vacuum energy to the complex s plane by

$$\mathcal{E}(s) = \frac{1}{s^{D/2}} \int_{p^2 < 1} \frac{d^D p}{(2\pi)^D} \sqrt{m^2 + p^2} \quad (2.22)$$

This is analytic throughout the complex s plane with the negative real axis removed because of the square root. For $|s|m^2 > 1$, it has a large s expansion identical to (2.21). Let C be a key-hole shaped contour which runs under the negative real axis up to $s = s_0$, ($s_0 > 1/m^2$), around the circle of radius s_0 centred on the origin and back to $s = -\infty$ running right above the negative real axis. Consider the integral

$$I(\lambda) = R(\lambda, s)\mathcal{E}(s) = \frac{1}{2\pi i} \int_C \frac{ds}{s} e^{\lambda s} \mathcal{E}(s) \quad (2.23)$$

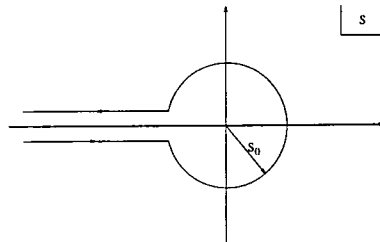


Figure 2.1: Contour of integration

The integral $\int_C e^s s^n ds$ is a representation of the factorial function [48] and evaluates to

$$\frac{1}{2\pi i} \int_C e^s s^n ds = \begin{cases} -\sin(n\pi)\Gamma(n + 1) & \text{if } n > 0 \\ 1/\Gamma(|n|) & \text{if } n < 0 \end{cases}$$

Therefore $I(\lambda)$ can be computed using the large s expansion to give

$$\sum_{n=0}^{\infty} \frac{\alpha_n}{\Gamma(n + 1 + D/2)} \left(\frac{\lambda}{m^2}\right)^{n+D/2} \quad (2.24)$$

Now the value of the integral does not change if we collapse the contour C to an arbitrarily small circle centred on $s = 0$ and a contour that just surrounds the negative real axis.

By taking λ to be real, positive and very large, the contribution from the negative real axis becomes exponentially suppressed away from the vicinity of the origin and thus the integral is determined for $\mathcal{E}(s)$ for small s . If the function $\mathcal{E}(s)$ was finite at the origin, we would have obtained $\mathcal{E}(0)$ up to exponentially suppressed terms.

An approximation scheme emerges if we truncate the series to a finite number of terms and work with a large value of λ . Since (2.24) is an alternating series, the error involved in truncating it to, say $n = N$, is less than the absolute value of the term $N + 1$, that is

$$\left| \frac{\alpha_{N+1} \lambda^{N+1+D/2}}{\Gamma(N+2+D/2) m^{2N+2+D}} \right| \quad (2.25)$$

which for large N behaves as $(e\lambda/m^2 N)^{(N+1+D/2)}/N$. Since we want to take λ large, let us set $\lambda = N\mu^2$. Then the truncation error goes to zero with large N provided the N -independent mass-scale μ is smaller than the particle mass m .

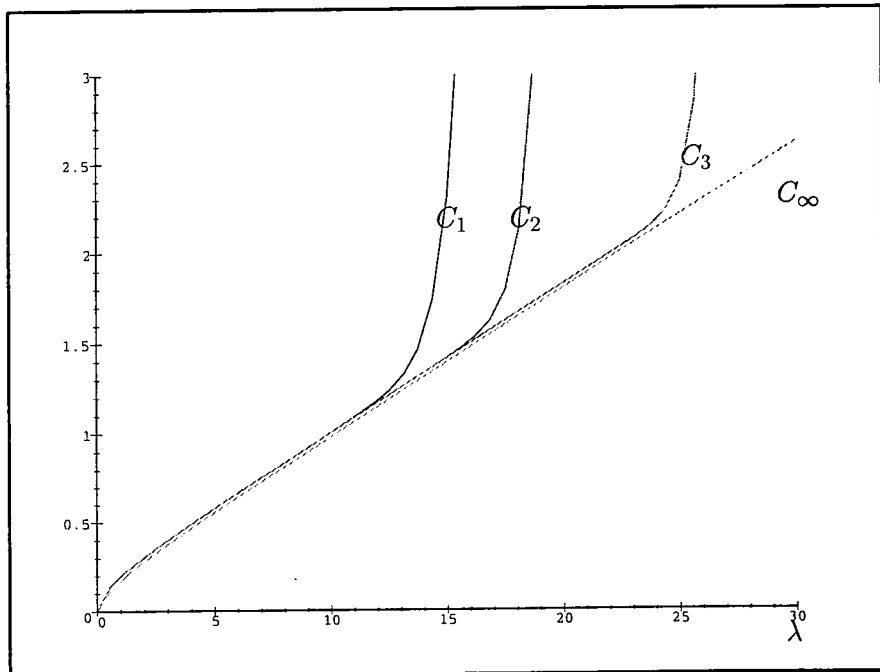


Figure 2.2: Resummation of the large s expansion

In figure(2.2) we plot the series (2.24) for $D = 1$ truncated to $n = 20$ (curve C_1), $n = 30$ (curve C_2) and $n = 50$ (curve C_3) so as to illustrate that the resummation of the large- s series (2.21) correctly reproduces the small- s behaviour of the energy density (2.20) which is expressed by curve C_∞ . The departure of the curves from the correct behaviour is because of the error involved in truncating the series to a certain order.

In summary, this shows that we can extract information about the high momentum cut-off theory by working to a finite order, N , with the local expansion of the vacuum functional valid for slowly varying fields. Using similar arguments, we now illustrate how the vacuum functional can be reconstructed from its large distance expansion.

Consider the $(1 + 1)$ -dimensional scalar theory. Define a scaled field $\varphi^s(x) = \varphi(\frac{x}{\sqrt{s}})$. We can prove that $W[\varphi^s]$ extends to an analytic function in the complex s plane with singularities only on the negative real axis (at least within an expansion in powers of φ).

First of all, in building up our proof it will be convenient to rotate coordinates in (2.6) in order to get a functional integral over the Euclidean space-time $x \geq 0, -\infty \leq t \leq \infty$:

$$e^{W[\varphi^s]} = \int \mathcal{D}\phi \ e^{-S_E^r + \int dt \phi'(0,t) \varphi^s(t)} \quad (2.26)$$

where the prime signifies a derivative with respect to x and S_E^r is the Euclidean action for the rotated space-time. This can be reinterpreted as the time ordered vacuum expectation value

$$T\langle 0^r | e^{\int dt \hat{\phi}'(0,t) \varphi^s(t)} | 0^r \rangle \quad (2.27)$$

where $|0^r\rangle$ is the ground state of the rotated Hamiltonian \hat{H}^r . If we expand the exponential in powers of φ^s and fourier transform the sources we get

$$\begin{aligned} \sum_n \int_{-\infty}^{+\infty} dt_n \int_{-\infty}^{t_n} dt_{n-1} \dots \int_{-\infty}^{t_2} dt_1 \frac{1}{(2\pi)^n} \int dk_n \dots dk_1 \exp(i \sum_i^n k_i t_i) \times \\ \tilde{\varphi}^s(k_n) \dots \tilde{\varphi}^s(k_1) \langle 0^r | \hat{\phi}'(0) e^{-(t_n - t_{n-1})\hat{H}^r} \hat{\phi}'(0) \\ \dots e^{-(t_3 - t_2)\hat{H}^r} \hat{\phi}'(0) e^{-(t_2 - t_1)\hat{H}^r} \hat{\phi}'(0) | 0^r \rangle. \end{aligned} \quad (2.28)$$

from which the time integrals can be computed. After some algebra we obtain the result

$$\begin{aligned} e^{W[\varphi^s]} = \sum_{n=0}^{\infty} \int dk_n \dots dk_1 \tilde{\varphi}(k_n) \dots \tilde{\varphi}(k_1) \delta(\sum_1^n k_i) \times \\ \sqrt{s}^n \langle 0^r | \hat{\phi}'(0) \frac{1}{\sqrt{s}\hat{H}^r + i(\sum_1^{n-1} k_i)} \hat{\phi}'(0) \dots \hat{\phi}'(0) \frac{1}{\sqrt{s}\hat{H}^r + ik_1} \hat{\phi}'(0) | 0^r \rangle. \end{aligned} \quad (2.29)$$

where we used that $\tilde{\varphi}^s(k) = \sqrt{s}\tilde{\varphi}(\sqrt{s}k)$. Now we take s to be complex. Since the eigenvalues of the Hamiltonian \hat{H}^r are real, the singularities occur for s on the negative real axis. The same holds for the connected part $W[\varphi^s]$ as any additional singularities could not cancel between connected and disconnected pieces.

A similar construction can be generalised to study the analyticity properties of the Yang-Mills vacuum functional in $3 + 1$ -dimensions. Following the same reasoning as for

the scalar field we can use the following functional representation of the Yang-Mills vacuum functional

$$\Psi[\mathbf{A}] = \int \mathcal{D}A e^{-S_E[A] - S_b[A, \mathbf{A}]} \quad (2.30)$$

where $S[A]$ is the Yang-Mills action in the Weyl gauge $A_0 = 0$ in the Euclidean space time with coordinates (\mathbf{x}, t) and $t \leq 0$,

$$S[A] = -\frac{1}{g^2} \int d^3\mathbf{x} dt tr \left(\dot{A}^2 + (\nabla \wedge A + A \wedge A)^2 \right). \quad (2.31)$$

The boundary term in the action is chosen to be

$$S_b[A, \mathbf{A}] = -\frac{2}{g^2} \int d^3\mathbf{x} tr \left((\mathbf{A} - A) \cdot \dot{A} \right) |_{t=0} \quad (2.32)$$

in order to satisfy some desired properties. We leave the boundary value of A to be freely integrated over, i.e. we will not impose a condition such as $A(\mathbf{x}, 0) = 0$ as we did for the scalar field. We will also assume that at spatial infinity the source \mathbf{A} is a pure gauge $\mathbf{A} \sim g(\hat{\mathbf{x}})^{-1} \nabla g(\hat{\mathbf{x}})$. Put this way, $\Psi[\mathbf{A}]$ is invariant under the gauge transformation $\delta_\omega \mathbf{A} = \nabla \omega + [\mathbf{A}, \omega]$, since the effect of varying the source \mathbf{A} may be compensated by gauge transforming A . As ω cannot depend on time, this is the residual gauge symmetry of $S[A]$ that preserves the gauge condition $A_0 = 0$. Moreover, functionally differentiating with respect to the source leads to an insertion of \dot{A} which, in Minkowskian time, leads to the Schrödinger representation of the canonical momentum represented by the non-Abelian electric field, $E = -ig^2 \delta / \delta \mathbf{A}$.

The only additional complication is that this time we have to work in three spatial dimensions. By studying separately the analyticity under complex scaling of the field in each dimension, it is easy to show that $\Psi[\mathbf{A}^s]$ for $\mathbf{A}^s(\mathbf{x}) = \frac{1}{\sqrt{s}} \mathbf{A}(\frac{1}{\sqrt{s}} \mathbf{x})$ continues to an analytic function of s on the complex plane with the negative real axis removed, just as in the scalar field theory case.

Having studied the analyticity properties of the W under complex scalings, we are ready to show how its local expansion, valid for slowly varying fields, can be used to construct the vacuum functional for arbitrary fields.

For a scalar field φ , define the integral

$$I(\lambda) \equiv \frac{1}{2\pi i} \int_C \frac{ds}{s-1} e^{\lambda(s-1)} W[\varphi^s], \quad (2.33)$$

where C is a very large circle centred on the origin in the complex s plane, beginning just below the negative real axis and ending just above. On C , the scaled field $\varphi^s(x) = \varphi(\frac{x}{\sqrt{s}}) \approx \varphi(0)$. Hence it varies slowly with x and we can use our local expansion. Now we can use the Cauchy theorem to relate the large s behaviour to the $s = 1$ value. If we collapse the contour to a small circle around $s = 1$, which contributes to $W[\varphi]$, and a contour C' surrounding the negative real axis, when $\Re(\lambda) > 0$ the latter is exponentially suppressed. In other words, for large $|s|$ we can use the local expansion and elsewhere on C' the integrand of (2.33) is bounded. Therefore we can formally write

$$W[\varphi] = \lim_{\lambda \rightarrow \infty} \frac{1}{2\pi i} \int_{|s| \rightarrow \infty} \frac{ds}{s-1} e^{\lambda(s-1)} W[\varphi^s] \quad (2.34)$$

which is expressed in terms of its local expansion. In practice, as we show in the next chapters, we can truncate the series to a finite number of terms and work with a finite value of λ to obtain a very good approximation.

For example, a local expansion of the vacuum functional for the 1 + 1-dimensional φ^4 theory written in terms of the scaled field is

$$\begin{aligned} W[\varphi^s] &= \int dx \left(a_1(\varphi^s)^2 + a_2(\varphi'^s)^2 + a_3(\varphi^s)^2(\varphi'^s)^2 + \dots \right) \\ &= \left(a_1\sqrt{s}\varphi^2 + a_2\frac{1}{\sqrt{s}}(\varphi')^2 + a_3\frac{1}{\sqrt{s}}(\varphi)^2(\varphi')^2 + \dots \right). \end{aligned} \quad (2.35)$$

This can be used to expand the vacuum functional $\Psi[\varphi^s]$ in inverse powers of $s - 1$, with coefficients that depend on the original configuration, say $\psi[\varphi]$, such that $\Psi[\varphi^s] \sim \sum (s - 1)^{-n} \psi[\varphi]$. Thus

$$S(\lambda) \equiv \frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s-1} e^{\lambda(s-1)} \Psi[\varphi^s] = \sum_n \frac{\lambda^n \psi[\varphi]}{\Gamma(n+1)} \quad (2.36)$$

and, for large λ ,

$$\Psi[\varphi] \approx \sum_n \frac{\lambda^n \psi[\varphi]}{\Gamma(n+1)}. \quad (2.37)$$

Let us illustrate that for the vacuum functional of a free massive scalar field theory in (1 + 1)-dimensions. The vacuum functional for the scaled field reads

$$\Psi[\varphi^s] = e^{-\frac{1}{2} \int dx \varphi \sqrt{-\nabla^2 + sm^2} \varphi} \quad (2.38)$$

which expanded in inverse powers of $(s - 1)$ yields the local series:

$$W[\varphi^s] = -\frac{m}{2} \sum_0^\infty \frac{\Gamma(3/2)}{\Gamma(n+1)\Gamma(3/2-n)} (s-1)^{1/2-n} \int dx \varphi \left(1 - \frac{\nabla^2}{m^2} \right)^n \varphi. \quad (2.39)$$

Also

$$\frac{1}{2\pi i} \int_C \frac{ds}{s-1} e^{\lambda(s-1)} W[\varphi^s] = \frac{m}{4\sqrt{\pi}} \sum_0^\infty \frac{(-)^n \lambda^{n-1/2}}{n!(n-1/2)} \int dx \varphi \left(1 - \frac{\nabla^2}{m^2}\right)^n \varphi \quad (2.40)$$

whose integrals exist for all n provided that the field has a momentum cut-off Λ but the integral will converge for all λ and Λ because of the $n!$ in the denominator. We can write (2.40) as

$$-\frac{m}{2\sqrt{\pi}} \int dx \varphi \left(\frac{1}{\sqrt{\lambda}} e^{-\lambda(1-\nabla^2/m^2)} + \int_0^\lambda d\lambda \frac{1}{\sqrt{\lambda}} e^{-\lambda(1-\nabla^2/m^2)} \left(1 - \frac{\nabla^2}{m^2}\right) \right) \varphi, \quad (2.41)$$

as one can check by expanding the exponentials, which is, in turn

$$-\frac{1}{2} \int dx \varphi \sqrt{-\nabla^2 + m^2} \varphi + \frac{m}{4\sqrt{\pi}} \int dx \varphi \left(\int_\lambda^\infty d\lambda \frac{1}{\sqrt{\lambda}^3} e^{-\lambda(1-\nabla^2/m^2)} \right) \varphi. \quad (2.42)$$

Notice that (2.42) tends to $W[\varphi]$ for $\lambda \rightarrow \infty$. Moreover, the error in expressing $W[\varphi]$ by the series (2.40) for λ large, is given by the last integral in (2.42) and is exponentially suppressed.

Chapter 3

A Schrödinger Equation for the Local Expansion

In constructing the Schrödinger equation satisfied by the local expansion of the vacuum functional, we have to bear in mind that short distance effects expressed by a cut-off are present, whereas our local expansion holds only for large distances. This apparent contradiction can be solved by scaling the cut-off as well as the field and using Cauchy's theorem to build the Schrödinger equation that acts directly on that local expansion. In this chapter we construct such a Schrödinger equation for the scalar ϕ_{1+1}^4 theory and set the grounds for its semi-classical solution.

3.1 Introduction

As we argued in the previous chapter, the logarithm of the vacuum functional of a quantum field theory is in general a non-local quantity. If the field varies slowly on the scale of the inverse of the mass of the lightest physical particle, it can be simplified to a local expansion which for a scalar theory in 1 + 1 dimensions we generically write as

$$W = \int dx \sum B_{j_0 \dots j_n} \varphi(x)^{j_0} \varphi'(x)^{j_1} \dots \varphi^{(n)}(x)^{j_n}. \quad (3.1)$$

The coefficients of this expansion $B_{j_0 \dots j_n}$ are constant if we assume translation invariance and finite as the ultraviolet cut-off is removed [5]. The knowledge of the local expansion was shown to be sufficient to reconstruct W for generic fields [3]. This is nice as we know that particle structure is characterised by length scales smaller than m_0^{-1} and so we could not use our local expansion to probe this scale. For this purpose, we have to know the $B_{j_0 \dots j_n}$ which are in principle computable from the Schrödinger equation that the vacuum

functional satisfies. However, as we have already learnt from the vacuum energy density for the free scalar field (see equations (2.20) and (2.21)), expanding in local quantities does not commute with removing the cut-off. In other words, the Schrödinger equation depends explicitly on short distance effects via the cut-off whereas our local expansion is only valid for fields characterised by large length scales. We cannot simply substitute the local expansion into the Schrödinger equation and expect to satisfactorily take the limit in which the cut-off is removed. To remedy this, we can again exploit the analyticity properties of the Schrödinger equation under complex scalings: by scaling the cut-off as well as the fields, the Schrödinger equation extends to an analytic function with cuts on the negative real axis. Thus, we can use Cauchy's theorem to build a version of the Schrödinger equation which can act directly on our local expansion [2],[4].

As a result, we show in this chapter that the eigenvalue problem of the Hamiltonian leads to an infinite set of algebraic equations for the coefficients $B_{j_0 \dots j_n}$. This set of equations can be solved in two approaches: the usual semi-classical expansion and a new approach, as proposed in [2], which does not rely on the smallness of the coupling constant and thus offers the possibility of solution beyond perturbation theory.

Clearly our framework has firstly to be tested within a semi-classical expansion so as to show that it is able to reproduce its standard results.

3.2 ϕ^4 Theory in $(1 + 1)$ -Dimensions

We adopt ϕ_{1+1}^4 as a toy theory to expose our arguments. It will be convenient in many ways. Obviously it turns out to be the simplest interacting theory capable of illustrating our framework. Furthermore, for φ_{3+1}^4 theory, Symanzik [5] proved that the Schrödinger wave functionals are finite as the cut-off is removed when they are constructed as functional integrals defined on a space-time with boundaries if, in addition to the usual renormalisation counterterms, a further field renormalisation is performed to take into account the divergences associated with the boundary. The surface counterterms were calculated within perturbation theory but since φ_{3+1}^4 is not asymptotically free, these are not reliable. So, we work, instead, in $(1 + 1)$ -dimensions where the theory is super-renormalisable and there are no further divergencies associated with the boundary, in which case there is no extra field renormalisation. Moreover, the laplacian, which requires point splitting already

for the free theory, in the renormalisable $(3 + 1)$ -dimensional interacting theory also involves factors that depend logarithmically on the point splitting distance, while no such factors are needed in either free field or super-renormalisable theory [52],[2]. This situation is not unrealistic since for Yang-Mills theories in four dimensions, there are no gauge invariant local counterterms on the three dimensional boundaries so that the renormalisation of the Schrödinger functional is the same as in the usual case without boundaries [7] and, in an asymptotically free theory, the behaviour of those logarithmic factors as the argument goes to zero can be obtained from the renormalisation group [51].

In a super-renormalisable theory, the number of divergent diagrams is finite. In the case of ϕ_{1+1}^4 , only mass renormalisation is required¹. There is only one mass counterterm due to the divergent tadpole diagram comprising the contribution to the self-energy of lowest order in the coupling constant. This mass counterterm can be evaluated analytically either in the framework of perturbation theory or, equivalently, by normal ordering the Hamiltonian with respect to the perturbative vacuum. In this task, we employ Wick's theorem: expanding the powers of the field in a sum of normal-ordered terms with more and more self contractions so as to separate the convergent term (with no contractions) from the divergent ones (with at least one contraction). The latter are just the negative of the required counterterms. Thus, we will be able to calculate the exact cut-off dependence of the renormalised parameters.

Let us start by writing the normal-ordered ϕ_{1+1}^4 Hamiltonian, represented by

$$: \hat{H} := \int dx : \left(\frac{1}{2} (\hat{\pi}(x)^2 + \hat{\varphi}'(x)^2 - M^2 \hat{\varphi}(x)^2) + \frac{g}{4!} \hat{\varphi}^4 \right) : . \quad (3.2)$$

In order to make explicit the cut-off dependence, define the Hamiltonian written for a momentum cut-off ϵ

$$\hat{H}_\epsilon = \int dx \left(\frac{1}{2} (\hat{\pi}_\epsilon + \hat{\varphi}_\epsilon'^2 + M^2(\epsilon) \hat{\varphi}_\epsilon^2) + \frac{g}{4!} \hat{\varphi}_\epsilon^4 - \mathcal{E}(\epsilon) \right) \quad (3.3)$$

where the cut-off fields are

$$\hat{\varphi}_\epsilon(x) = \int dy \mathcal{G}_\epsilon(x, y) \hat{\varphi}(y), \quad \hat{\pi}_\epsilon(x) = \int dy \mathcal{G}_\epsilon(x, y) \hat{\pi}(y)$$

with the momentum cut-off

$$\mathcal{G}_\epsilon(x, y) = \int_{p^2 < 1/\epsilon} \frac{dp}{2\pi} e^{ip(x-y)} \quad (3.4)$$

¹In addition, we have to subtract the constant infinite zero-point contribution from the Hamiltonian.

According to our plan, we want to define divergent quantities $M^2(\epsilon)$ and $\mathcal{E}(\epsilon)$ such that $\lim_{\epsilon \rightarrow 0} \hat{H}_\epsilon \Psi = \hat{H} \Psi$. We write

$$T_\epsilon \equiv \langle 0 | \hat{\varphi}_\epsilon(x) \hat{\varphi}_\epsilon(x) | 0 \rangle = \frac{1}{2} \int_{p^2 < 1/\epsilon} \frac{dp}{2\pi} \frac{1}{\sqrt{p^2 + M^2}} \quad (3.5)$$

to formally represent the logarithmically divergent tadpole in 1 + 1-dimensions which coincides with the vacuum expectation value of φ^2 or a self contraction of the field. Next we rewrite \hat{H}_ϵ as

$$\hat{H}_\epsilon = \int dx \left(\frac{1}{2} (\hat{\pi}_\epsilon + \hat{\varphi}_\epsilon'^2 + M^2 \hat{\varphi}_\epsilon^2) + \frac{1}{2} (M^2(\epsilon) - M^2) \hat{\varphi}_\epsilon^2 + \frac{g}{4!} \hat{\varphi}_\epsilon^4 - \mathcal{E}(\epsilon) \right), \quad (3.6)$$

and we call the free part as

$$\hat{H}_\epsilon^0 = \int dx \left(\frac{1}{2} (\hat{\pi}_\epsilon + \hat{\varphi}_\epsilon'^2 + M^2 \hat{\varphi}_\epsilon^2) \right) \quad (3.7)$$

which if normal-ordered yields

$$: \hat{H}_\epsilon^0 := \hat{H}_\epsilon^0 - \frac{1}{2} \int_{p^2 < 1/\epsilon} \frac{dp}{2\pi} \omega_p, \quad (3.8)$$

$\omega_p = \sqrt{p^2 + M^2}$, i.e. the subtraction of the constant infinite zero point energy. The next step is to write the product of fields in terms of normal ordered quantities

$$\begin{aligned} \frac{1}{2} (M^2(\epsilon) - M^2) \varphi_\epsilon^2 + \frac{g}{4!} \varphi_\epsilon^4 &= \frac{1}{2} (M^2(\epsilon) - M^2) (: \varphi_\epsilon^2 : + T_\epsilon) + \frac{g}{4!} (: \varphi_\epsilon^4 : + 6T_\epsilon : \varphi_\epsilon^2 : + 3T_\epsilon^2) \\ &= \frac{1}{2} \left((M^2(\epsilon) - M^2) + \frac{g}{2} T_\epsilon \right) : \varphi_\epsilon^2 : + \frac{g}{4!} : \varphi_\epsilon^4 : + \frac{(M^2(\epsilon) - M^2)}{2} T_\epsilon + \frac{g}{8} T_\epsilon^2 \end{aligned} \quad (3.9)$$

Now substituting (3.7), (3.8) and (3.9) into (3.6), enables us write

$$\begin{aligned} \hat{H}_\epsilon &= \int dx \left(: \hat{H}_\epsilon : + \frac{1}{2} \int_{p^2 < 1/\epsilon} \frac{dp}{2\pi} \omega_p + \frac{1}{2} (M^2(\epsilon) - M^2) (: \hat{\varphi}_\epsilon^2 : + T_\epsilon) \right. \\ &\quad \left. + \frac{g}{4!} (6T_\epsilon : \varphi_\epsilon^2 : + 3T_\epsilon^2) - \mathcal{E}(\epsilon) \right). \end{aligned} \quad (3.10)$$

where $: \hat{H}_\epsilon := : \hat{H}_\epsilon^0 : + g/4! : \hat{\varphi}_\epsilon^4 :$, from which we calculate the exact cut-off dependence of $M(\epsilon)$ and $\mathcal{E}(\epsilon)$ to be

$$M^2(\epsilon) = M^2 + \hbar \delta M^2 - \hbar \frac{g}{4} \int_{p^2 < 1/\epsilon} \frac{dp}{2\pi} \frac{1}{\sqrt{p^2 + M^2}}, \quad (3.11)$$

$$\mathcal{E}(\epsilon) = \delta \mathcal{E} + \frac{\hbar}{2} \int_{p^2 < 1/\epsilon} \frac{dp}{2\pi} \left(\sqrt{p^2 + M^2} + \frac{M^2(\epsilon) - M^2}{2\sqrt{p^2 + M^2}} \right) + \frac{g\hbar^2}{32} \left(\int_{p^2 < 1/\epsilon} \frac{dp}{2\pi} \frac{1}{\sqrt{p^2 + M^2}} \right)^2, \quad (3.12)$$

In (3.11) and (3.12), we made explicit the \hbar dependence and represented the ambiguity in the choice of the counterterms (subtraction point) by δM^2 and $\delta \mathcal{E}$ which is resolved, as usual, by renormalisation conditions ².

² $\mathcal{E}, M^2, \delta \mathcal{E}$ and δM^2 remain finite as the cut-off is removed.

3.3 A Set of Independent Local Functionals

The most general local derivative expansion for the vacuum functional of a scalar interacting theory is (3.1). We further assume parity invariance and that $\varphi \rightarrow -\varphi$ is an unbroken symmetry of the Lagrangian which restricts both the total number of φ 's and the total number of derivatives to be even. Moreover, the expansion functions $\varphi^{j_0} \varphi^{j_1} \varphi^{j_2} \dots$, are related by partial integration so we can specify a linearly independent basis by insisting that the power of the highest derivative be at least two³. So, for example, $\int dx \varphi(x) \varphi''(x) (\varphi'''(x))^2$ is a basis vector but neither $\int dx \varphi^2(x) (\varphi''(x))^3$ nor $\int dx \varphi(x)^3 \varphi''(x)$ are basis vectors. The former breaks $\varphi \rightarrow -\varphi$ symmetry and the latter, since the power of the highest derivative is one, can be reduced to a basis vector by means of integration by parts, namely $\int dx \varphi(x)^2 (\varphi'(x))^2$. A basis vector so defined cannot be reduced to another basis vector by partial integration and therefore we have a well defined basis.

3.4 The Schrödinger Equation

Having defined the Hamiltonian for ϕ_{1+1}^4 theory (3.6), we proceed to construct the Schrödinger equation satisfied by the vacuum functional, which we express as $\exp(W[\varphi]/\hbar)$. In the coordinate Schrödinger representation, the canonical momentum is represented by a functional differentiation $\hat{\pi} = -i\hbar\delta/\delta\varphi(x)$, so the kinetic term leads to the product of two functional derivatives at the same point which we regulate by introducing a momentum cut-off $p^2 < 1/\epsilon$.

The Schrödinger equation is $\lim_{\epsilon \rightarrow 0} F_\epsilon[\varphi] = 0$ where

$$F_\epsilon[\varphi] = -\frac{\hbar}{2} \Delta_\epsilon W + \int dx \left(\frac{1}{2} \left(-\left(\frac{\delta W}{\delta \varphi} \right)^2 + \varphi'^2 + M^2(\epsilon) \varphi^2 \right) + \frac{g}{4!} \varphi^4 - \mathcal{E}(\epsilon) \right) \quad (3.13)$$

and

$$\Delta_\epsilon = \int dx dy \int_{p^2 < 1/\epsilon} \frac{dp}{2\pi} e^{ip(x-y)} \frac{\delta^2}{\delta\varphi(x)\delta\varphi(y)} = \int_{p^2 < 1/\epsilon} dp 2\pi \frac{\delta^2}{\delta\tilde{\varphi}(-p)\delta\tilde{\varphi}(p)}, \quad (3.14)$$

where $\tilde{\varphi}(p) = \int dx \varphi(x) \exp(-ipx)$.

Suppose that we evaluate $F_\epsilon[\varphi]$ for slowly varying φ , i.e. a φ whose fourier transform is non-zero only for momenta less than m_0 , the mass of the lightest physical particle, say.

³We can formally prove it by induction [53].

Then it will reduce to a sum of local functionals of φ :

$$F_\epsilon[\varphi] = \int dx \sum f_{j_0 \dots j_n}(\epsilon) \varphi(x)^{j_0} \varphi'(x)^{j_1} \dots \varphi^{(n)}(x)^{j_n} \quad (3.15)$$

It is important to notice that (3.15) is not the same expression that would be obtained if we acted Δ_ϵ on the local expansion (3.1). The former correctly includes differentiation with respect to the fourier modes of φ with momenta in the range $m_0^2 < p^2 < 1/\epsilon$, absent from the latter.

The solution to this problem is to scale the cut-off $\epsilon \rightarrow \epsilon s$ as well as the field $\varphi(x) \rightarrow \varphi^s(x) \equiv \varphi(\frac{x}{\sqrt{s}})$. Doing so, $(\Delta_{s\epsilon} W)[\varphi_s]$ (see appendix A), as well as $M^2(s\epsilon)$ and $\mathcal{E}(s\epsilon)$ extend to an analytic function in the complex s plane with singularities lying on the negative real axis and the same is true of the coefficients of the linearly independent expansion functions, $f_{j_0 \dots j_n}$ in (3.15). Therefore, the contour integral

$$I_{j_0 \dots j_n}(\lambda) = \frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s} e^{\lambda s} f_{j_0 \dots j_n}(s\epsilon) \quad (3.16)$$

can be calculated by collapsing the contour to a small circle about the origin and a contour along the cut on the negative real axis. Let us call the latter as contour C . When $|s|$ is large, the scaled field φ_s is slowly varying and the scaled cut-off $1/(s\epsilon)$ is less than m_0 . Therefore $(\Delta_{s\epsilon} W)[\varphi_s]$ can be calculated by acting with $\Delta_{s\epsilon}$ directly on the local expansion of W , (3.1). Furthermore, as the real part of λ tends to infinity, the contribution from the cut tends to zero due to the $\exp(\lambda s)$ factor. The contribution from the circle about the origin is controlled by the small ϵ behaviour of $f_{j_0 \dots j_n}(\epsilon)$. As $\epsilon \rightarrow 0$ this vanishes due to the Schrödinger equation and, in perturbation theory, the Feynman diagram expansion gives an asymptotic expansion of $f_{j_0 \dots j_n}(\epsilon s)$ in positive powers of $\sqrt{\epsilon s}$, namely

$$f_A(\epsilon s) = f_A^0 + f_A^1 \sqrt{\epsilon s} + f_A^2 \epsilon s + f_A^3 (\sqrt{\epsilon s})^3 + \dots \quad (3.17)$$

where A expresses a group of indices and f_A^i some dimensionful constants. The action of the resummation operator $R(\lambda, s) = 1/(2\pi i) \int_C ds \exp(\lambda s)/s$ on (3.17) yields

$$f_A^0 + f_A^1 \sqrt{\epsilon} \frac{1}{\sqrt{\pi \lambda}} + 0 + f_A^3 \sqrt{\epsilon}^3 \left(\frac{-1}{2\sqrt{\pi}} \right) \frac{1}{\lambda^{\frac{3}{2}}} + \dots \quad (3.18)$$

Thus, if instead of simply $R(\lambda, s)f_A(\epsilon s)$ we use $(R(\lambda, s)\sqrt{\pi \lambda s})f_A(\epsilon s)$ we have

$$f_A^0 + 0 + f_A^2 \epsilon \left(\frac{-1}{2} \right) \frac{1}{\lambda} + \dots \quad (3.19)$$

from which we conclude that the inclusion of $\sqrt{\pi\lambda s}$ in (3.16) will ensure that the contribution from the origin will be of order $1/\lambda$ rather than $1/\sqrt{\lambda}$ which will improve our resummation. Henceforth we redefine (3.16) as

$$I_{j_0\dots j_n}(\lambda) = \frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s} e^{\lambda s} \sqrt{\pi\lambda s} f_{j_0\dots j_n}(s\epsilon). \quad (3.20)$$

As the product $s\epsilon$ now plays the rôle of cut-off, rather than ϵ alone, we take ϵ to be finite and equal to unity.

The Schrödinger equation leads to an infinite set of algebraic equations expressed by

$$\lim_{\lambda \rightarrow \infty} I_{j_0 j_1 \dots j_n}(\lambda) = 0 \quad (3.21)$$

where

$$\begin{aligned} I_0 &= -\bar{\mathcal{E}}(\lambda) - \hbar \frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(B_2 + \frac{B_{0,2}\lambda}{3} + \frac{B_{0,0,2}\lambda^2}{10} + \dots \right) \\ I_2 &= \frac{\bar{M}^2(\lambda)}{2} - 2B_2^2 - \hbar \frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(6B_4 + \frac{B_{2,2}\lambda}{3} + \frac{B_{2,0,2}\lambda^2}{10} + \dots \right) \\ I_4 &= \frac{g}{4!} - 8B_2B_4 - \hbar \frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(15B_6 + \frac{B_{4,2}\lambda}{3} + \frac{B_{4,0,2}\lambda^2}{10} + \dots \right) \\ I_{0,2} &= \frac{1}{2} - 4B_2B_{0,2} - \hbar \frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(B_{2,2} + 2B_{0,4}\lambda + \frac{4B_{2,0,2}\lambda^2}{3} + \dots \right) \\ I_{0,0,2} &= \frac{32B_2B_{0,0,2} + 16B_{0,1}^2}{3} - \hbar \frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(-B_{2,0,2} + \left(\frac{B_{1,0,3}}{3} - \frac{B_{0,4}}{9} \right) \lambda + \dots \right) \end{aligned}$$

...

$$\begin{aligned} I_{0,\dots,j_n=2} &= \sum_{m \geq 3} \frac{4\sqrt{\pi} B_{0,0,\dots,j_n=2} B_{0,0,\dots,j_n-m=2}}{\Gamma(n+1/2)} - \hbar \frac{\sqrt{\lambda}}{\sqrt{\pi}} \times \\ &\times \left(-\frac{2B_{2,0,\dots,j_n=2}}{\Gamma(n+1)} + \frac{2(B_{1,0,1,0,\dots,j_n=2} - B_{0,2,0,\dots,j_n=2})\lambda^{\frac{3}{2}}}{3\Gamma(n+2)} + \dots \right) \end{aligned}$$

...

$$\begin{aligned} I_{2k} &= \sum_{n=0}^{k-1} \tilde{B}_{(0,n)} \tilde{B}_{(0,k-(n+1))} (n-k)(n+1) - \hbar \frac{\sqrt{\lambda}}{\sqrt{\pi}} \times \\ &\times \left(2(k+1)(2k+1) \tilde{B}_{(0,k)} + \sum_{n=1} \rho(n) \tilde{B}_{(n,k)} \lambda^n \right) \quad k \geq 3. \end{aligned} \quad (3.22)$$

...

with

$$\bar{\mathcal{E}}(\lambda) = \frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s} e^{\lambda s \sqrt{\pi \lambda s}} \mathcal{E}(s) = \sum_0^{\infty} \hbar^n \bar{\mathcal{E}}(\lambda)^{\hbar^n}, \quad (3.23)$$

$$\bar{M}^2(\lambda) = \frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s} e^{\lambda s \sqrt{\pi \lambda s}} M^2(s) = M^2 + \hbar \bar{M}^2(\lambda)^{\hbar}. \quad (3.24)$$

Also, for the ease of notation, in the last line of (3.22) we call $\tilde{B}_{(r,s)}$ the coefficients in the subset

$$\tilde{W} = \sum_{r,s} \int dx \tilde{B}_{(r,s)} \varphi^{2r} \varphi^{(s)^2} \quad (3.25)$$

of W , which in our usual notation rewrite

$$\tilde{B}_{(r,s)} = B_{2r,0,\dots,j_s=2}, \tilde{B}_{(r,0)} = B_{2r+2} \quad (3.26)$$

and $\rho(n) = 2/(\Gamma(n+1)(2n+1))$.

In appendix B, we show a computer programme which constructs the $I_{j_0\dots j_n}$ given the local expansion as an input.

Summarizing, we have an equation for the coefficient of each independent local function of φ (basis vectors). An approximation scheme emerges from working to a finite order in λ and taking λ large, but finite, in the same fashion as we did for the vacuum energy density of the free scalar theory. These equations may be solved semi-classically by first ignoring the power series in λ . This amounts to ignoring the laplacian in the Schrödinger equation (3.13) and solving the resulting Hamilton-Jacobi equation as a local expansion. This local expansion is possible because the full solution for the Hamilton-Jacobi equation is the Euclidean action on shell and the classical theory is massive. We can iteratively compute the quantum corrections to the coefficients by substituting the leading order values into $\Delta_s W$.

3.5 The Hamilton-Jacobi Equation

We proceed to study some properties of the equations which determine the leading order values of the coefficients $B_{j_0 j_1 \dots j_n}$. Neglecting the \hbar -dependent terms in (3.22) amounts to solve the so called Hamilton-Jacobi equation for a local expansion in the fields, from which one can obtain the classical values of the coefficients of such expansion.

For the φ^4 scalar field theory in two dimensions, the Euclidean action reads

$$S_E = \int d^2 x \mathcal{L}_E(\varphi, \partial_\mu \varphi) \quad (3.27)$$

and the Hamilton-Jacobi equation for a time-independent potential is

$$H\left(\frac{\delta S_E}{\delta\varphi}, \varphi\right) = 0, \quad (3.28)$$

with the Euclidean Lagrangian density given by

$$\mathcal{L}_E = \frac{1}{2}(\dot{\varphi}^2 + \varphi'^2) + \frac{1}{2}M^2\varphi^2 + \frac{g}{4!}\varphi^4 \quad (3.29)$$

and

$$\begin{aligned} \mathcal{H} &= \pi\dot{\varphi} - \mathcal{L}_E = \frac{1}{2}\pi^2 - V_0(\varphi), \\ V_0(\varphi) &= \frac{\varphi'^2}{2} + \frac{1}{2}M^2\varphi^2 + \frac{g}{4!}\varphi^4, \end{aligned} \quad (3.30)$$

so that (3.28) becomes

$$\frac{1}{2}\left(\frac{\delta S_E}{\delta\varphi}\right)^2 - V_0(\varphi) = 0. \quad (3.31)$$

If we expand W in the vacuum functional $\Psi = e^W$ in a \hbar -series

$$W = \sum_{n=0} \hbar^{n-1} W_n, \quad (3.32)$$

the equation (3.13) to order \hbar^0 collapses to

$$\int dx \left(\frac{1}{2} \left(\frac{\delta W_0}{\delta\varphi} \right)^2 - V_0(\varphi) \right) = 0 \quad (3.33)$$

which tells us that W_0/\hbar can be represented by S_E as expected. If we evaluate the Hamilton-Jacobi equation for the scaled field φ^s then for large s the field varies slowly in space. So we can employ the local expansion (3.1) to obtain a set of linear algebraic equations for the (classical) coefficients $B_{j_0 j_1 \dots j_n}$ which is just the $O(\hbar^0)$ pieces of the equations (3.22) that from now on we call $I_{j_0 j_1 \dots j_n}^0$, and then use the analyticity properties to obtain an approximate vacuum functional for arbitrary φ as we described in the previous chapter.

3.5.1 Some Particular Leading Order Coefficients

Let us examine in more detail the subset of independent local functionals of the form (3.25) as it will be possible to obtain analytic formulae for the leading order coefficients $\tilde{B}_{(r,s)}^0$ ⁴ defined as (3.26). This is because the $O(\hbar^0)$ system of equations which determine such coefficients comprises only terms of the form $\tilde{B}_{(i,j)}^0$.

⁴The superscript 0 denotes a $O(\hbar^0)$ quantity.

The classical equations are basically determined by $\int dx (\delta W/\delta\varphi(x))^2$. An exercise of integration by parts shows that the $O(\hbar^0)$ equation correspondent to $\int dx \varphi^{2m}\varphi^{(n)^2}$,

$$\tilde{I}_{(m,n)}^0 = 0, \quad (3.34)$$

contain only terms coming from similar local functionals, that is from

$$\mathcal{P}(k_1, l_1, k_2, l_2) \equiv \tilde{B}_{(k_1, l_1)}^0 \tilde{B}_{(k_2, l_2)}^0 \left(\frac{\delta}{\delta\varphi(z)} \int \varphi^{2k_1} \varphi^{(l_1)^2} \right) \cdot \left(\frac{\delta}{\delta\varphi(z)} \int \varphi^{2k_2} \varphi^{(l_2)^2} \right). \quad (3.35)$$

In determining a particular $\tilde{I}_{(m,n)}^0$ from $\int dz \sum_{k_1, l_1, k_2, l_2} \mathcal{P}(k_1, l_1, k_2, l_2)$, we constrain (3.35) to yield the same number of fields and number of derivatives,

$$2m + 2 = 2k_1 + 2 - 1 + 2k_2 + 2 - 1 \Rightarrow m = k_1 + k_2 \quad (3.36)$$

and

$$2l_1 + 2l_2 = 2n \Rightarrow l_1 + l_2 = n. \quad (3.37)$$

Using

$$\frac{\delta}{\delta\varphi(z)} \int dx \varphi^{2k} \varphi^{(l)^2} = 2k\varphi^{2k-1} \varphi^{(l)^2} + 2(-)^l \frac{d^l}{dx^l} (\varphi^{2k} \varphi^{(l)})_{x=z} \quad (3.38)$$

and

$$\frac{d^n}{dx^n} (A(x)B(x)) = \sum_{k=0}^n \binom{n}{k} A^{(n-k)}(x) B^{(k)}(x) \quad (3.39)$$

we can show that

$$\begin{aligned} \mathcal{P}(k_1, l_1, k_2, l_2) = & 4 \left(k_1 k_2 \varphi^{2k_1-1} \varphi^{2k_2-1} \varphi^{(l_1)^2} \varphi^{(l_2)^2} + \right. \\ & \left. + k_2 (-)^{l_1} \varphi^{2k_2-1} \varphi^{(l_2)^2} \sum_{i=0}^{l_1} \binom{l_1}{i} (\varphi^{2k_1})^{(l_1-i)} \varphi^{(l_1+i)} + (1 \leftrightarrow 2) + \right. \\ & \left. + (-1)^n \sum_{i=0}^{l_1} \binom{l_1}{i} (\varphi^{2k_1})^{(l_1-i)} \varphi^{(l_1+i)} \sum_{j=0}^{l_2} \binom{l_2}{j} (\varphi^{2k_2})^{(l_2-j)} \varphi^{(l_2+j)} \right) \tilde{B}_{(k_1, l_1)}^0 \tilde{B}_{(k_2, l_2)}^0 \end{aligned} \quad (3.40)$$

and thus

$$\left(\int dz \varphi^{2m} \varphi^{(n)^2} \right) \tilde{I}_{(m,n)}^0 = \int dz \sum_{k_1, l_1} \mathcal{P}(k_1, l_1, m - k_1, n - l_1) = 0 \quad (3.41)$$

where we should also include terms from the classical potential V^0 when it is the case.

We are ready to determine $\tilde{I}_{(m,n)}^0$ by examining the terms shown in (3.40). The first term is $k_1 k_2 \varphi^{2m-2} \varphi^{(l_1)^2} \varphi^{(l_2)^2}$ and contributes to $\tilde{I}_{(m,n)}^0$ only if $l_1 = 0$ or $l_1 = n \Rightarrow l_2 = 0$ as

$$\int dz \varphi^{2m}(z) \varphi^{(n)^2}(z) \sum_{k_1} k_1 (m - k_1) \left(\tilde{B}_{(k_1, 0)}^0 \tilde{B}_{(m-k_1, n)}^0 + \tilde{B}_{(k_1, n)}^0 \tilde{B}_{(m-k_1, 0)}^0 \right). \quad (3.42)$$

In the second term, if $l_2 \neq 0$, the only contribution comes from $l_2 = n$, that is

$$\int dz \varphi^{2m}(z) \varphi^{(n)^2}(z) \sum_{k_1} (m - k_1) \tilde{B}_{(k_1,0)}^0 \tilde{B}_{(m-k_1,n)}^0, \quad (3.43)$$

and if $l_2 = 0$, it becomes

$$k_2 (-)^n \varphi^{2k_2+1} \sum_{i=0}^n \binom{n}{i} (\varphi^{2k_1})^{(n-i)} \varphi^{(n+i)} \quad (3.44)$$

which contributes to $\tilde{I}_{(m,n)}^0$ with

$$\int dz \varphi^{2m}(z) \varphi^{(n)^2}(z) \sum_{k_1} \left(\sum_{i=0}^{n-1} \binom{n}{i} (-)^{i+n} 2k_1 (m - k_1) + (m - k_1)(2m + 1) \right) \tilde{B}_{(k_1,n)}^0 \tilde{B}_{(m-k_1,0)}^0 \quad (3.45)$$

and the third term (which is obtained from the second by interchanging the indices $1 \leftrightarrow 2$) contributes with a similar term. The last term contributes according to the value of l_1 .

If $l_1 = 0$ it gives

$$\int dz \varphi^{2m}(z) \varphi^{(n)^2}(z) \sum_{k_1} \left(\sum_{j=0}^{n-1} \binom{n}{j} (-)^{j+n} 2(m - k_1) + (2m + 1) \right) \tilde{B}_{(k_1,0)}^0 \tilde{B}_{(m-k_1,n)}^0 \quad (3.46)$$

whereas if $l_1 = n$ we have

$$\int dz \varphi^{2m}(z) \varphi^{(n)^2}(z) \sum_{k_1} \left(\sum_{i=0}^{n-1} \binom{n}{i} (-)^{i+n} 2k_1 + (2m + 1) \right) \tilde{B}_{(k_1,n)}^0 \tilde{B}_{(m-k_1,0)}^0 \quad (3.47)$$

and finally for $0 < l_1 < n$ the only contribution is of the form

$$\int dz \varphi^{2m}(z) \varphi^{(n)^2}(z) \sum_{k_1, l_1} \tilde{B}_{(k_1, l_1)}^0 \tilde{B}_{(m-k_1, n-l_1)}^0. \quad (3.48)$$

The calculation above is important to test the results of our computer programme which includes calculating $\int (\delta W / \delta \varphi)^2$ from a general set of local independent functionals W and then a routine for integration by parts and reduction to a basis vector element (see appendix B).

The set of equations of the form $\tilde{I}_{(i,j)}^0$ can be systematically solved to render analytical formulae for all the leading order coefficients of the form $\tilde{B}_{(m,n)}^0$ defined by (3.25). For example, the classical equations which determine the $\tilde{B}_{(0,n)}^0$, can be written as

$$\tilde{I}_{(0,n)}^0 = \sum_{k=0}^n \tilde{B}_{(0,k)}^0 \tilde{B}_{(0,n-k)}^0 \quad (3.49)$$

for $k \geq 2$. The coefficients $\tilde{B}_{(0,0)}^0$ and $\tilde{B}_{(0,1)}^0$ are determined by the equations I_2 and $I_{0,2}$ in (3.22):

$$\begin{aligned} \frac{M}{2} - 2(\tilde{B}_{(0,0)}^0)^2 &= 0 \\ \frac{1}{2} - 4\tilde{B}_{(0,0)}^0 \tilde{B}_{(0,1)}^0 &= 0 \end{aligned} \quad (3.50)$$

which give $\tilde{B}_{(0,0)}^0 = -1/2$ ⁵ and $\tilde{B}_{(0,1)}^0 = -1/4$, where we have adopted a mass scale so that $M = 1$. We can write (3.49) in a power series form as

$$\left(\sum_{n=0}^{\infty} \tilde{B}_{(0,n)}^0 z^n \right)^2 = (\tilde{B}_{(0,0)}^0)^2 + 2\tilde{B}_{(0,0)}^0 \tilde{B}_{(0,1)}^0 z \quad (3.51)$$

by the vanishing of each coefficient of z , and hence solve for $\tilde{B}_{(0,n)}^0$ to give

$$\tilde{B}_{(0,n)}^0 = -\frac{1}{2} \binom{1/2}{n} \quad n = 2, 3, 4, \dots \quad (3.52)$$

In this way, we have determined all the classical values for the expansion coefficients

$\int dx \tilde{B}_{(0,n)}^0 \varphi^{(n)2}$. It will also be useful to determine $\int dx \tilde{B}_{(1,n)}^0 \varphi^2 \varphi^{(n)2}$. Equation I_4 in (3.22) determines $\tilde{B}_{(1,n)}^0 = -g/96$ whereas for $n = 1, 2, 3, \dots$, we have to solve the equations

$$\begin{aligned} \tilde{I}_{(1,1)}^0 &\equiv 2\tilde{B}_{(0,0)}^0 \tilde{B}_{(1,1)}^0 + 6\tilde{B}_{(0,1)}^0 \tilde{B}_{(1,0)}^0 = 0, \\ \tilde{I}_{(1,2)}^0 &\equiv 2\tilde{B}_{(0,0)}^0 \tilde{B}_{(1,2)}^0 + \tilde{B}_{(0,1)}^0 \tilde{B}_{(1,1)}^0 + 6\tilde{B}_{(0,2)}^0 \tilde{B}_{(1,0)}^0 = 0, \\ \tilde{I}_{(1,3)}^0 &\equiv 2\tilde{B}_{(0,0)}^0 \tilde{B}_{(1,3)}^0 + \tilde{B}_{(0,1)}^0 \tilde{B}_{(1,2)}^0 + \tilde{B}_{(0,2)}^0 \tilde{B}_{(1,1)}^0 + 6\tilde{B}_{(0,3)}^0 \tilde{B}_{(1,0)}^0 = 0, \end{aligned} \quad (3.53)$$

etc.. If we redefine

$$\begin{aligned} \tilde{B}_{(0,0)}^0 &\rightarrow \frac{1}{2} \tilde{B}_{(0,0)}^0, \\ \tilde{B}_{(1,0)}^0 &\rightarrow \frac{1}{6} \tilde{B}_{(1,0)}^0, \end{aligned} \quad (3.54)$$

equation (3.53) becomes

$$\begin{aligned} \tilde{B}_{(0,0)}^0 \tilde{B}_{(1,1)}^0 + \tilde{B}_{(0,1)}^0 \tilde{B}_{(1,0)}^0 &= 0, \\ \tilde{B}_{(0,0)}^0 \tilde{B}_{(1,2)}^0 + \tilde{B}_{(0,1)}^0 \tilde{B}_{(1,1)}^0 + \tilde{B}_{(0,2)}^0 \tilde{B}_{(1,0)}^0 &= 0, \\ \tilde{B}_{(0,0)}^0 \tilde{B}_{(1,3)}^0 + \tilde{B}_{(0,1)}^0 \tilde{B}_{(1,2)}^0 + \tilde{B}_{(0,2)}^0 \tilde{B}_{(1,1)}^0 + \tilde{B}_{(0,3)}^0 \tilde{B}_{(1,0)}^0 &= 0, \end{aligned} \quad (3.55)$$

which, in turn, can again be expressed as the vanishing of each coefficient of z in the product of the power series:

$$\left(\sum_{n=0}^{\infty} \tilde{B}_{(0,n)}^0 z^n \right) \left(\sum_{m=0}^{\infty} \tilde{B}_{(1,m)}^0 z^m \right) = \tilde{B}_{(0,0)}^0 \tilde{B}_{(1,0)}^0. \quad (3.56)$$

We can solve for $\tilde{B}_{(1,m)}^0$ by using the standard formulae of inversion and product of power series [49], which yields, after undoing (3.54),

$$\tilde{B}_{(1,n)}^0 = -\frac{g}{16} \begin{vmatrix} \tilde{B}_{(0,1)}^0 & \tilde{B}_{(0,2)}^0 & \cdots & \tilde{B}_{(0,n-1)}^0 & \tilde{B}_{(0,n)}^0 \\ -1 & \tilde{B}_{(0,1)}^0 & \cdots & \tilde{B}_{(0,n-2)}^0 & \tilde{B}_{(0,n-1)}^0 \\ 0 & -1 & \cdots & \tilde{B}_{(0,n-3)}^0 & \tilde{B}_{(0,n-2)}^0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & \tilde{B}_{(0,1)}^0 \end{vmatrix} \quad (3.57)$$

⁵We took the negative root for normalisability.

and therefore we were able to find a formula for $\tilde{B}_{(1,n)}^0$ in terms of $\tilde{B}_{(1,0)}^0 = -g/96$ and the previous $\tilde{B}_{(0,n)}^0$ which are known to be (3.52). In a similar fashion we can find the the classical coefficients of $\int dx \tilde{B}_{(2,n)}^0 \varphi^4 \varphi^{(n)^2}$. The equations which determine such coefficients are

$$\begin{aligned} \tilde{I}_{(2,0)}^0 &\equiv 2(\tilde{B}_{(1,0)}^0)^2 + 3\tilde{B}_{(2,0)}^0 \tilde{B}_{(0,0)}^0 = 0, \\ \tilde{I}_{(2,1)}^0 &\equiv 16\tilde{B}_{(1,0)}^0 \tilde{B}_{(1,1)}^0 + 6\tilde{B}_{(0,0)}^0 \tilde{B}_{(2,1)}^0 + 30\tilde{B}_{(0,1)}^0 \tilde{B}_{(2,0)}^0 = 0, \\ \tilde{I}_{(2,2)}^0 &\equiv 16\tilde{B}_{(1,0)}^0 \tilde{B}_{(1,2)}^0 + (\tilde{B}_{(1,1)}^0)^2 + 6\tilde{B}_{(0,0)}^0 \tilde{B}_{(2,2)}^0 + \tilde{B}_{(0,1)}^0 \tilde{B}_{(2,1)}^0 + 30\tilde{B}_{(0,2)}^0 \tilde{B}_{(2,0)}^0 = 0, \\ \tilde{I}_{(2,3)}^0 &\equiv 16\tilde{B}_{(1,0)}^0 \tilde{B}_{(1,3)}^0 + 2\tilde{B}_{(1,1)}^0 \tilde{B}_{(1,2)}^0 + 6\tilde{B}_{(0,0)}^0 \tilde{B}_{(2,3)}^0 + 2\tilde{B}_{(0,1)}^0 \tilde{B}_{(2,2)}^0 \\ &\quad + 2\tilde{B}_{(0,2)}^0 \tilde{B}_{(2,1)}^0 + 30\tilde{B}_{(0,3)}^0 \tilde{B}_{(2,0)}^0 = 0, \end{aligned} \quad (3.58)$$

etc. , which if this time we redefine

$$\begin{aligned} \tilde{B}_{(0,0)}^0 &\rightarrow \frac{1}{3} \tilde{B}_{(0,0)}^0, \\ \tilde{B}_{(1,0)}^0 &\rightarrow \frac{1}{8} \tilde{B}_{(1,0)}^0, \\ \tilde{B}_{(2,0)}^0 &\rightarrow \frac{1}{15} \tilde{B}_{(2,0)}^0, \end{aligned} \quad (3.59)$$

allows us to write those equations as

$$\left(\sum_{n=0}^{\infty} \tilde{B}_{(1,n)}^0 z^n \right)^2 + 2 \left(\sum_{m=0}^{\infty} \tilde{B}_{(0,m)}^0 z^m \right) \left(\sum_{l=0}^{\infty} \tilde{B}_{(2,l)}^0 z^l \right) - (\tilde{B}_{(1,0)}^0)^2 - 2\tilde{B}_{(0,0)}^0 \tilde{B}_{(2,0)}^0 = 0 \quad (3.60)$$

where each coefficient of z must separately vanish. If we set $\left(\sum_{m=0}^{\infty} \tilde{B}_{(0,m)}^0 z^m \right)^{-1} = \sum_{m=0}^{\infty} \beta_m z^m$ as well as $\left(\sum_{n=0}^{\infty} \tilde{B}_{(1,n)}^0 z^n \right)^2 = \sum_{n=0}^{\infty} \gamma_n z^n$ we can formally write, after substituting back the original values of $\tilde{B}_{(0,0)}^0$, $\tilde{B}_{(1,0)}^0$ and $\tilde{B}_{(2,0)}^0$,

$$\begin{aligned} \tilde{B}_{(2,n)}^0 &= \frac{1}{2} \left((\tilde{B}_{(1,0)}^0)^2 + 2\tilde{B}_{(0,0)}^0 \tilde{B}_{(2,0)}^0 \right) \beta_n - \frac{1}{2} \sum_{k=0}^n \beta_k \gamma_{n-k} \\ &= -\frac{1}{2} \left(\frac{1}{27648} \beta_n + \sum_{k=0}^n \beta_k \gamma_{n-k} \right), \end{aligned} \quad (3.61)$$

$n \geq 1$. Using the formulae for inversion and product of power series from the mathematical literature [49], we can calculate all the $\tilde{B}_{(2,n)}^0$.

3.6 Solving the Schrödinger equation

As we have discussed earlier, the equations (3.22) can be solved to determine the coefficients B_{j_0, \dots, j_n} within the standard semi-classical scheme. Clearly a loop expansion

amounts to a weak coupling expansion: one can rescale the field so that the factor appearing in the path integral is $1/(g^2\hbar)$ that is

$$\frac{S}{\hbar} \rightarrow \frac{S}{g^2\hbar} . \quad (3.62)$$

Then, if we expand the logarithm of the vacuum functional in powers of \hbar like

$$W = \sum_{n=0} \hbar^{n-1} W^{\hbar^n}, \quad W^{\hbar^0} \equiv W^0, \quad (3.63)$$

the Schrödinger equation to $O(\hbar)$ is written as $\lim_{\epsilon \rightarrow 0} F_\epsilon^{\hbar}[\varphi] = 0$ with

$$F_\epsilon^{\hbar}[\varphi] = \hbar \left(\frac{1}{2} \Delta_\epsilon W^0 + \int dx \left(\frac{\delta W^0}{\delta \varphi} \right) \left(\frac{\delta W^{\hbar}}{\delta \varphi} \right) - V_\epsilon^{\hbar} \right), \quad (3.64)$$

where

$$\begin{aligned} V_\epsilon^{\hbar} &= \int dx \frac{1}{2} M^2(\epsilon)^{\hbar} \varphi^2(x) - \mathcal{E}(\epsilon)^{\hbar} \\ W^{\hbar}[\varphi] &= \sum \int dx B_{j_0, \dots, j_n}^{\hbar} \varphi^{j_0}(x) \dots (\varphi^{(n)})^{j_n}, \end{aligned} \quad (3.65)$$

which illustrates that quantum corrections to the coefficients B_{j_0, \dots, j_n} can be obtained iteratively by substituting the leading order solutions into the laplacian.

For theories which are massless at the classical level, the semi classical approach is not applicable within our framework. Notwithstanding, if there is quantum mechanical generation of mass, as is believed to be the case for some theories of physical interest like Yang-Mills, then our local expansion does make sense (for fields that vary slowly on the scale of the lightest glueball, in the case of Yang-Mills theory) but another method than the semi-classical approach has to be employed to solve the resulting algebraic equations.

In [2] it was suggested a new method to solve these equations which basically consists of truncating the expansion in λ for each linear independent expansion function at certain order, say λ^N , the error being estimated by studying the asymptotic behaviour of $\Delta_s W$ for large s and N using equation (A.18). In this approach there is no expansion parameter as the approximation consists of working with a large but finite value of N and λ and therefore it is a non-perturbative scheme since it does not rely on the smallness of the coupling constant.

Finally the particle spectrum can also be calculated in a similar fashion [2]. The one-particle wave functional corresponding to the lightest physical particle in the theory can

be thought to have the form of a pre-factor P multiplying the vacuum functional Ψ . For slowly varying fields, it can be written as an integral of a local function

$$P = \int dx (\varphi + a_1 \varphi^3 + a_2 \varphi^5 + \dots + b_1 \varphi \varphi'^2 + b_2 \varphi \varphi'^4 + \dots + c_1 \varphi^3 \varphi'^2 + \dots). \quad (3.66)$$

The Schrödinger equation which determines these expansion coefficients is linear in P

$$\frac{1}{2\pi i} \int_c ds \frac{e^{\lambda s}}{s} \left(\frac{1}{2} \Delta_s P + \int dx \frac{\delta P}{\delta \varphi(x)} \frac{\delta W}{\delta \varphi(x)} + m P \right) \quad (3.67)$$

and in principle can also be solved by the method proposed in [2].

Chapter 4

Short Distance Properties from Large Distance Behaviour

It is important to show that our framework effectively reproduces the results that can be obtained within the standard approach of semi-classical expansion. In particular, since physical states are built out of their large distance behaviour, it is crucial to verify if this formalism correctly incorporates the short distance behaviour as contained in the counterterms of the Hamiltonian, which we demonstrate in this chapter. We also point out a curious simplification valid for the Sine-Gordon and Sinh-Gordon wave functional and illustrate how the vacuum functional can be reconstructed from its local expansion valid for slowly varying fields.

4.1 Introduction

We are discussing an approach to quantum field theory in which the physical states are constructed out of their large distance expansion. We showed in the previous chapter that such expansion for the vacuum functional satisfies its particular form of the Schrödinger equation from which the expansion coefficients can be calculated, for example, within the standard semi-classical expansion. We have also seen that from the knowledge of its local expansion, valid only for slowly varying fields on the scale of the inverse of the mass of the lightest physical particle in the theory, it is possible to reconstruct the vacuum functional for an arbitrary field configuration using its analyticity properties under complex scaling. Furthermore a new scheme, originally proposed in [2], offers the possibility of solution beyond perturbation theory in the couplings for the expansion coefficients. However,

before this is attempted, it is essential to demonstrate that our formalism, which starts off with a large distance expansion, gets the right short distance behaviour as is contained in the counterterms present in the hamiltonian. In other words, we want to study how the renormalisation of the ultraviolet (short distance) infinities are described in our approach which we will illustrate in the context of ϕ_{1+1}^4 theory.

In the previous chapter we determined the explicit cut-off dependence of the counterterms for ϕ_{1+1}^4 theory, expressed by the relations (3.11) and (3.12). The ambiguity in the choice of the counterterms represented by δM^2 and $\delta \mathcal{E}$ is to be resolved, as usual, by renormalisation conditions. There is a natural way to do this in our context. Notice that the counterterms only enter I_0 and I_2 in (3.22). If these are fixed then these equations determine the coefficients B_{j_0, \dots, j_n} and the energy eigenvalue, \mathcal{E} , which are themselves finite as the cut-off is removed. Alternatively we could choose the values of two of these quantities, B_2 and \mathcal{E} for example, and then think of the equations $I_0 = 0$ and $I_2 = 0$ as determining the counter-terms. So we will take

$$B_2 = -\frac{M}{2}, \quad (4.1)$$

which is its classical value, and

$$\mathcal{E} = 0 \quad (4.2)$$

as our renormalisation conditions. The advantage of imposing the renormalisation conditions on \mathcal{E} and B_2 is that we are free to solve (3.22) for the remaining B_{j_0, \dots, j_n} without first computing the λ -dependence of the counter-terms which in a more general context can only be done in perturbation theory.

4.2 The Mass Subtraction

In the semi-classical approach, the equations (3.22) may be solved by first ignoring the terms proportional to \hbar in order to calculate the leading order coefficients B_{j_0, \dots, j_n}^0 . Although the resulting equations are quadratic in these coefficients they are readily solved by starting with the coefficients of local functions of the lowest dimension and number of φ . In chapter 3 we showed how to get exact formulae for the leading order coefficients of local functions of the form $\int dx \varphi^{2n}(x) \varphi^{(m)^2}(x)$ and gave explicit expressions for $B_{0,0, \dots, 0, j_n=2}^0$, $B_{2,0, \dots, 0, j_n=2}^0$ and $B_{4,0, \dots, 0, j_n=2}^0$ (please see equations (3.52), (3.57) and (3.61)). With the

help of our computer programme showed in appendix B, we could also solve the resulting equations which determine the leading order coefficients of more generic basis functions.

Thus we can write, to leading order ¹

$$\begin{aligned}
W_{tree} = \int dx \left(-\frac{1}{2}\varphi^2 - \frac{1}{4}\varphi'^2 + \frac{1}{16}\varphi''^2 - \frac{1}{32}\varphi'''^2 + \frac{5}{256}\varphi''''^2 - \frac{1}{96}g\varphi^4 + \frac{1}{64}g\varphi^2\varphi'^2 \right. \\
- \frac{1}{128}g\varphi^2\varphi''^2 + \frac{1}{256}g\varphi'^4 + \frac{5}{1024}g\varphi^2\varphi'''^2 - \frac{3}{256}g\varphi\varphi''^3 - \frac{31}{1024}g\varphi'^2\varphi''^2 \\
\left. - \frac{7}{2048}g\varphi^2\varphi''''^2 + \frac{41}{1024}g\varphi\varphi''\varphi'''^2 + \frac{75}{2048}g\varphi'^2\varphi'''^2 - \frac{93}{4096}g\varphi''^4 + \dots \right) \quad (4.3)
\end{aligned}$$

We start by showing that our large distance expansion correctly gives the short distance behaviour as contained in the divergent mass subtraction given by $\bar{M}^2(\lambda)$ which occur only in I_2 (3.22). Using the values which we have calculated for $B_{2,0,\dots,0,j_n=2}^0$ we get the $O(\hbar)$ expression

$$I_2^\hbar(\lambda) = \frac{\bar{M}^2(\lambda)^\hbar}{2} + 2B_2^\hbar - g\frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(\frac{1}{16} - \frac{\lambda}{192} + \frac{\lambda^2}{1280} - \frac{5\lambda^3}{43008} + \dots \right) \quad (4.4)$$

where $\bar{M}^2(\lambda)^\hbar$, as given by (3.24), is expressed by

$$\bar{M}^2(\lambda)^\hbar \equiv \delta M^2 - g\frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(\frac{1}{4} + \sum_{m=0} (-1)^{m+1} \mathcal{F}(m) \lambda^{m+1} \right), \quad (4.5)$$

with

$$\mathcal{F}(m) = \frac{\Gamma(m+3/2)}{4\sqrt{\pi}(2m+3)(\Gamma(m+2))^2}. \quad (4.6)$$

The RHS of equation (4.4) vanishes as $\lambda \rightarrow \infty$ but in the spirit of our method we hope to get a good approximation if we truncate the series and take λ as large as the truncation will allow, i.e. small enough for the first neglected term to be insignificant.

Now since $I(\lambda)$ is of order $1/\lambda$ for large λ (3.19), the accuracy of this approximation is greatly improved if we perform a further contour integration, amounting to a resummation of the series in λ . Notice that if we substitute $\lambda = 1/\sqrt{s}$ in (4.4), $I_2^\hbar(1/\sqrt{s})$ is a function that is analytic in s with a cut on the negative real axis that we wish to evaluate as s tends to zero from real positive values. Thus we define

$$\tilde{I}(\lambda) = \frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s} e^{\lambda^2 s \sqrt{\pi \lambda^2 s}} I(s^{-1/2}) \quad (4.7)$$

for which $\lim_{\lambda \rightarrow \infty} \tilde{I}(\lambda) = 0$ and hence, to order \hbar , (4.7) translates into

$$\tilde{I}^\hbar(\lambda) = \frac{\delta M^2 + \bar{M}^2(\lambda)^\hbar}{2} + 2B_2^\hbar - gS(\lambda) \quad (4.8)$$

¹We have chosen our mass scale so that $M = 1$.

where

$$S(\lambda) = \frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(\frac{1}{16\Gamma(3/4)} - \frac{\lambda\sqrt{2}\Gamma(3/4)}{96\pi} + \frac{\lambda^2}{960\Gamma(3/4)} - \frac{\lambda^3\sqrt{2}\Gamma(3/4)}{5376\pi} + \dots \right) \quad (4.9)$$

and

$$\tilde{M}^2(\lambda)^{\hbar} = -g \frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(\frac{\sqrt{2}\Gamma(1/4)}{8} + \sum_{m=0} (-1)^{m+1} \pi \frac{\mathcal{F}(m)}{\Gamma((m+2)/2 + 1/4)} \lambda^{m+1} \right) \quad (4.10)$$

The terms in $S(\lambda)$ now decrease more rapidly than the corresponding terms in $I(\lambda)$. Since $I(1/\sqrt{s})$ behaves asymptotically as \sqrt{s} for small s this resummation has the effect of eliminating the leading term so that $\tilde{I}(\lambda)$ is now of order $1/\lambda^2$. Further resummations are only efficacious given a sufficient number of terms in the truncated series for the extra gamma functions in the coefficients to be noticeable.

In fig.(4.1) we plot, the series $S(\lambda)$ truncated to 13 terms, $-\tilde{M}^2(\lambda)^{\hbar}/(2g)$, their sum, and the limit of this sum as $\lambda \rightarrow \infty$, (which we obtain exactly in the section 4.5 as $-1/(8\pi) \simeq -0.0398$).

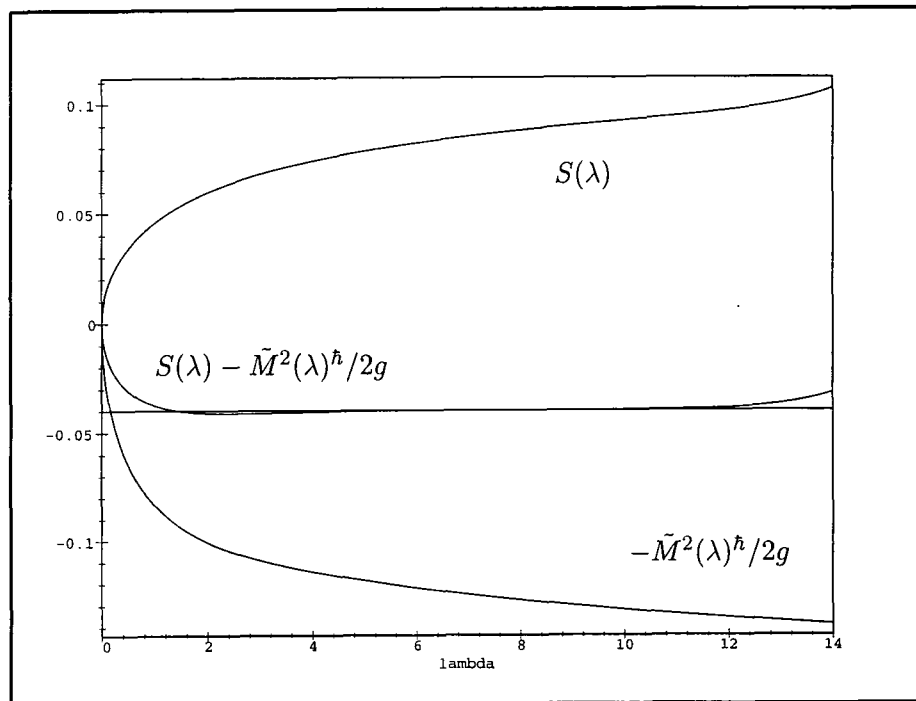


Figure 4.1: The Mass Subtraction

Clearly neither $S(\lambda)$ nor $-\tilde{M}^2(\lambda)^{\hbar}/(2g)$ are constant for large λ but their sum is, to a good approximation for $\lambda > 2$. This shows that our large-distance expansion correctly

reproduces the short-distance effects encoded in $M^2(\epsilon)^{\hbar}$. The departure from this constant value for $\lambda > 11$ is due to the error involved in truncating the alternating series $S(\lambda)$ to 13 terms.

If we denote by S_n the $S(\lambda)$ series truncated to n terms minus $\tilde{M}^2(\lambda)^{\hbar}/(2g)$ then in fig.(4.2) we show S_n for $n = 4, 5, 8, 9, 12, 13$. This figure illustrates the resummation process and is a high-resolution plot of fig.(4.1), so to speak. Notice that $S(\lambda)$ being an alternating series, the direction of the departure of a curve from the correct value is associated with taking an even or odd number of terms in this series.

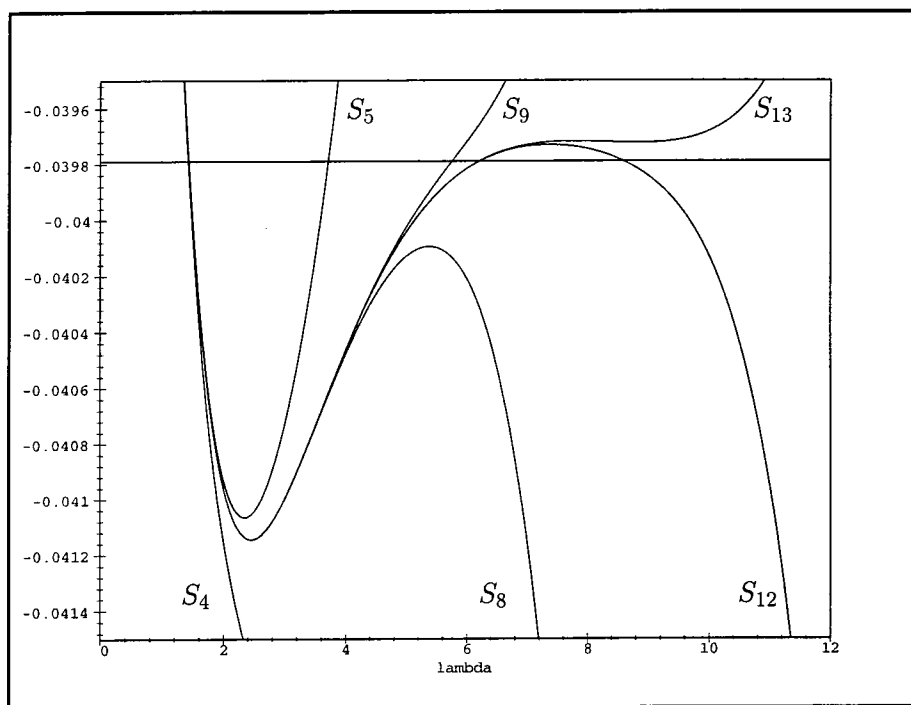


Figure 4.2: Truncating $S(\lambda)$

Each truncation provides a good approximation to $S(\lambda)$ up to a value of λ which is large enough for the highest order term to be a significant fraction of the whole. Taking this to be one per cent gives an estimate of $S(\infty)$ with an error that ranges from three per cent (five terms) to half a per cent (13 terms).

4.3 The Energy Subtraction

We proceed to check that our large distance expansion correctly reproduces the energy subtraction which is expressed by the equation $I_0 = 0$ in (3.22),

$$I_0 = -\bar{\mathcal{E}}(\lambda) - \hbar \frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(B_2 + \frac{B_{0,2}\lambda}{3} + \frac{B_{0,0,2}\lambda^2}{10} + \dots + \frac{1}{\Gamma(n+1)(2n+1)} B_{0,0,\dots,j_n=2} + \dots \right). \quad (4.11)$$

To order $O(\hbar)$, it can be written as

$$I_0^{\hbar}(\lambda) = -\bar{\mathcal{E}}^{\hbar}(\lambda) + \hbar \frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(\sum_{n=0} \frac{1}{2} \binom{1/2}{n} \frac{\lambda^n}{\Gamma(n+1)(2n+1)} \right) \equiv -\bar{\mathcal{E}}^{\hbar}(\lambda) + \hbar \bar{S}^{\hbar}(\lambda) \quad (4.12)$$

where, from (3.23),

$$\bar{\mathcal{E}}^{\hbar}(\lambda) = \frac{1}{2\pi i} \int_{|s|=\infty} ds \frac{e^{\lambda s}}{s} \sqrt{\lambda \pi s} \left(\frac{1}{2} \int_{p^2 < 1/s} \frac{dp}{2\pi} \sqrt{p^2 + 1} \right). \quad (4.13)$$

In fig.(4.3) we plot $-\bar{\mathcal{E}}^{\hbar}(\lambda)$, $\bar{S}^{\hbar}(\lambda)$ truncated to 12 terms, and their sum as expressed in (4.12) which vanishes as it should, reflecting the normal-ordering of the Hamiltonian. The departure from 0 at $\lambda = 8$ again reflects that we have truncated the series.

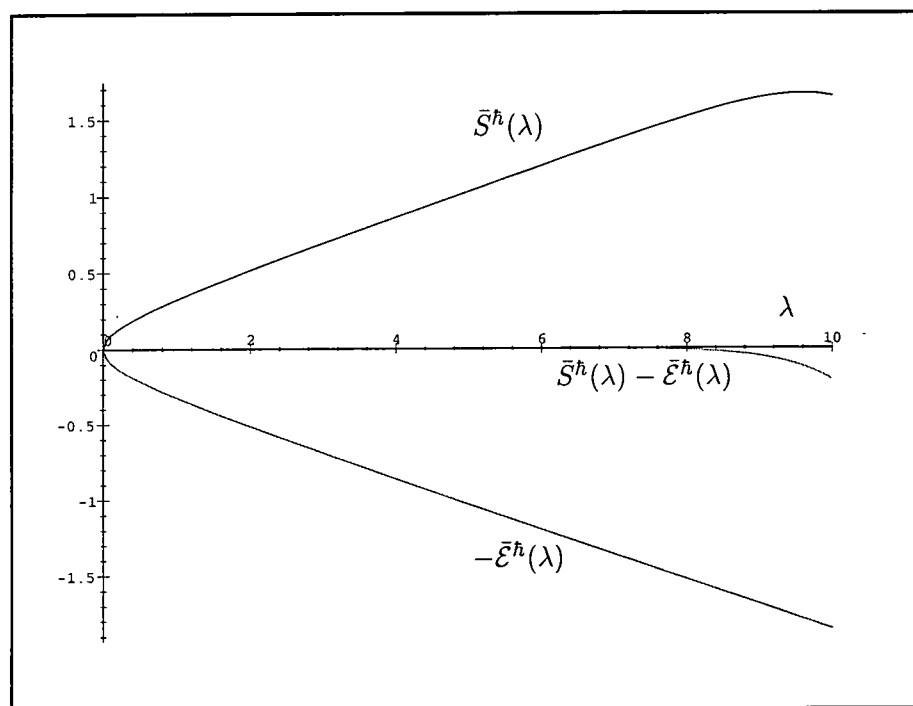


Figure 4.3: The $O(\hbar)$ Energy Subtraction

In order to analyse the $O(\hbar^2)$ energy subtraction, we need to calculate the $O(\hbar)$ part of $W[\varphi]$ that is quadratic in φ . We obtain this from the equations $I_{0,2} = 0, I_{0,0,2} = 0, \dots$,

having imposed the renormalisation condition $B_2 = -M/2$. For example, in determining $B_{0,2}^{\hbar}$, the first order correction of the coefficient of $\int dx \varphi'^2(x)$, we have to solve the equation

$$I_{0,2}^{\hbar} = 4(B_2 B_{0,2}^{\hbar}) + \hbar \frac{\sqrt{\lambda}}{\sqrt{\pi}} \left(B_{2,2}^0 + 2B_{0,4}^0 \lambda + \frac{4}{3} B_{2,0,2}^0 \lambda + \dots \right) \quad (4.14)$$

(see (3.64)).

We use the re-summation described earlier, truncate the series in λ so that they include contributions from coefficients of functionals of φ of dimension less than 26, and take λ so that the last included term is one per cent of the value of the truncated series [4]. We also use Stieltje's trick of halving the contribution of the last included term to improve the accuracy of the approximation [54]. This gives the estimate

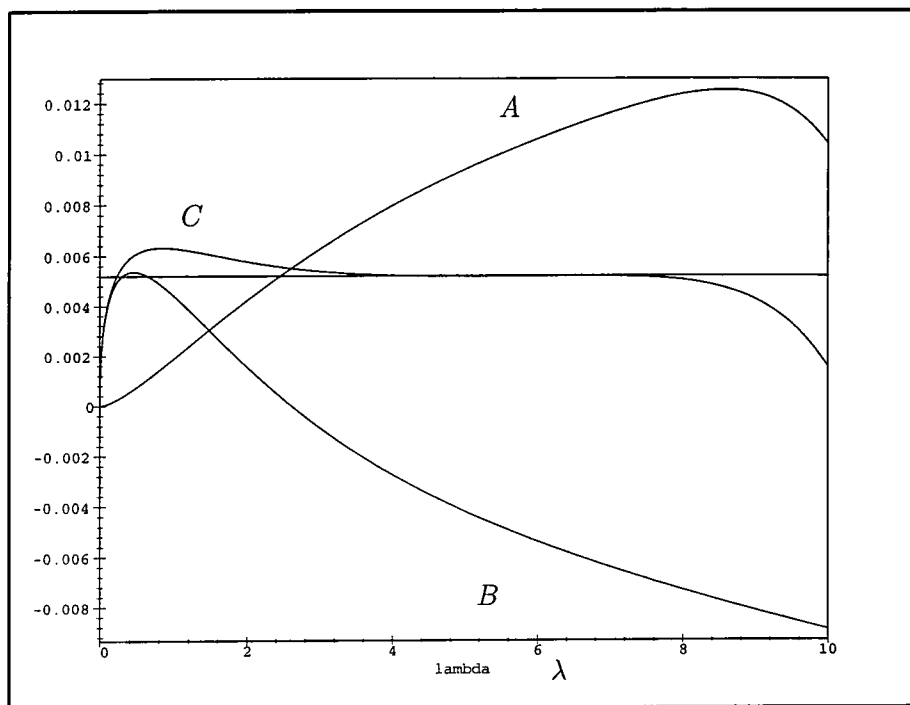
$$W_2^{\hbar} = \frac{g}{1000} \int dx \left(6.64\varphi'^2 - 6.02\varphi''^2 + 5.40\varphi'''^2 - 4.91\varphi''''^2 + 4.54\varphi^{(5)2} \right. \\ \left. - 4.24\varphi^{(6)2} + 4.01\varphi^{(7)2} - 3.79\varphi^{(8)2} + 3.58\varphi^{(9)2} - 3.34\varphi^{(10)2} + \dots \right) \quad (4.15)$$

In the next sections, we obtain W_2^{\hbar} exactly. Rounding the exact results to three significant figures gives

$$W_2^{\hbar} = \frac{g}{1000} \int dx \left(6.63\varphi'^2 - 5.97\varphi''^2 + 5.33\varphi'''^2 - 4.84\varphi''''^2 + 4.45\varphi^{(5)2} \right. \\ \left. - 4.14\varphi^{(6)2} + 3.89\varphi^{(7)2} - 3.68\varphi^{(8)2} + 3.50\varphi^{(9)2} - 3.34\varphi^{(10)2} + \dots \right) \quad (4.16)$$

which shows that our approximate results are good to a few per cent.

Figure (4.4) shows the effect of substituting this estimate into the $O(\hbar^2)$ contribution to I_0 . The top curve, A , is the estimate of the re-summation of the series in λ , whilst the bottom curve, B , is the $O(\hbar^2)$ contribution to the re-summation of $\bar{\mathcal{E}}(\lambda)$ evaluated using (3.12) with $\delta M^2 = g/(4\pi)$. Neither of these curves appears to tend to a constant for large λ whereas their sum, represented by the middle curve, C , provides a good approximation to a constant value for λ larger than four until λ is sufficiently large that the approximation of the infinite series by just ten terms breaks down. The straight line in the figure is the value 0.0052 which would be obtained by truncating the series at fifty terms using the expression for W_2^{\hbar} which we will present later.

Figure 4.4: The $O(\hbar^2)$ Energy Subtraction

4.4 Four Field Terms

Having proved that our large distance expansion correctly reproduces the short distance effects present in the counterterms of the Hamiltonian, we can proceed to evaluate the one loop correction to the expansion coefficients of higher number of fields. For the coefficients of local functions containing four fields, we start by calculating their leading order values which are obtained, as we have described before, by neglecting the $O(\hbar)$ part of the equations (3.22). Such equations can be obtained with the help of the computer programme (appendix B) and readily solved to give

$$W_4^0 = \frac{g}{1000} \int dx \left(-10.4\varphi^4 + 15.6\varphi^2\varphi'^2 + 3.91\varphi'^4 - 7.81\varphi^2\varphi''^2 - 30.3\varphi'^2\varphi''^2 - 11.7\varphi\varphi''^3 + 4.88\varphi^2\varphi'''^2 - 22.7\varphi''^4 + 36.6\varphi'^2\varphi'''^2 + 40.0\varphi\varphi''\varphi'''^2 - 3.42\varphi^2\varphi''''^2 + \dots \right) \quad (4.17)$$

Following the same reasoning as we described for the calculation of the two-field terms, the $O(\hbar)$ contribution is ([4])

$$W_4^{\hbar} = \frac{g^2}{10000} \int dx \left(4.02\varphi^4 - 20.0\varphi^2\varphi'^2 - 7.96\varphi'^4 \right)$$

$$\begin{aligned}
& +17.4\varphi^2\varphi''^2 + 83.8\varphi'^2\varphi''^2 + 37.6\varphi\varphi''^3 - 15.6\varphi^2\varphi'''^2 + 87.7\varphi''^4 \\
& \quad -129\varphi'^2\varphi'''^2 - 164\varphi\varphi''\varphi'''^2 + 14.0\varphi^2\varphi''''^2 + \dots \quad (4.18)
\end{aligned}$$

There are things to note. Firstly there is a proliferation of local functionals of the same dimension and number of φ as these increase. So, for example, there is a unique local functional with just two φ for any dimension, but there are two hundred and seven with twelve φ and dimension twelve. Secondly the ratio of the $O(\hbar)$ corrections to any two coefficients of functionals containing the same number of φ and the same dimension is approximately the same as the ratio of the tree-level values [4]. For example the ratio of the $O(\hbar)$ coefficients of $\varphi^2\varphi''^2$ and φ'^4 is $-17.4/7.96 \simeq -2.19\dots$ whereas the ratio of the corresponding tree-level values is exactly -2 . Given that our estimate is probably only good to a few per cent it is not clear at this stage whether the one-loop ratios are exactly equal to the tree-level ratios, but we will investigate this with greater accuracy in the next section. We will now compare these results with those obtained by solving the Schrödinger equation without first expanding in terms of local functions which is fairly easy to solve for low orders of an expansion in powers of φ and \hbar .

4.5 Direct Semi-Classical Solution

The Schrödinger equation $\lim_{\epsilon \rightarrow 0} F_\epsilon[\varphi] = 0$ can be solved without resorting to a local expansion in the fields. In this section we compute some exact formulae for the coefficients of two and four field basis functions in order to evaluate the precision of our method.

Let us expand the logarithm of the vacuum functional as

$$W[\varphi] = \sum_{n=1}^{\infty} \int dp_1 \dots dp_{2n} \tilde{\varphi}(p_1) \dots \tilde{\varphi}(p_{2n}) \Gamma_{2n}(p_1, \dots, p_{2n}) \delta(p_1 + \dots + p_{2n}) \quad (4.19)$$

where the Γ are unknown functions ².

The action of the laplacian on (4.19) is symbolically expressed by $\Delta_\epsilon W[\varphi] = \sum \Delta \Gamma_{2n}$ where $\Delta \Gamma_{2n}$ is

$$\int_{q^2 < 1/\epsilon} 2\pi dq \int dp_3 \dots dp_{2n} 2n(2n-1) \tilde{\varphi}(p_3) \dots \tilde{\varphi}(p_{2n}) \Gamma_{2n}(q, -q, p_3, \dots, p_{2n}) \delta(p_3 + \dots + p_{2n}). \quad (4.20)$$

²We have derived a formal expression for Γ (equation (2.29) with $s = 1$) but here we will expand it in powers of \hbar .

Likewise, we write

$$\int dx \left(\frac{\delta W}{\delta \varphi} \right)^2 = \int dp (2\pi) \frac{\delta W}{\delta \tilde{\varphi}(p)} \frac{\delta W}{\delta \tilde{\varphi}(-p)} \equiv \sum_{n,m} \Gamma_{2n} \circ \Gamma_{2m} \quad (4.21)$$

with $\Gamma_{2n} \circ \Gamma_{2m}$ equal to

$$8mn\pi \int dp_2 \dots dp_{2n} dk_2 \dots dk_{2m} \tilde{\varphi}(p_2) \dots \tilde{\varphi}(p_{2n}) \tilde{\varphi}(k_2) \dots \tilde{\varphi}(k_{2m}) \delta(p_2 + \dots + p_{2n} + k_2 + \dots + k_{2m}) \\ \times \Gamma_{2n}(-(p_2 + \dots + p_{2n}), p_2, \dots, p_{2n}) \Gamma_{2m}(-(k_2 + \dots + k_{2m}), k_2, \dots, k_{2m}) \quad (4.22)$$

We want to find the Γ 's for a certain number of fields in (4.19) as an expansion in powers of \hbar . Let

$$\Gamma_{2n} = \sum_{m=0} \hbar^m \Gamma_{2n}^{\hbar^m}, \quad \Gamma_{2n}^{\hbar^0} \equiv \Gamma_{2n}^0, \quad (4.23)$$

To tree level, the Schrödinger equation yields

$$\Gamma_2^0 \circ \Gamma_2^0 + 2\Gamma_2^0 \circ \Gamma_4^0 + 2\Gamma_2^0 \circ \Gamma_6^0 + \Gamma_4^0 \circ \Gamma_4^0 + \dots = \int dx \left(\varphi'^2 + M^2 \varphi^2 + \frac{g}{12} \varphi^4 \right). \quad (4.24)$$

The term quadratic in φ is

$$\Gamma_2^0 \circ \Gamma_2^0 = \int dp 8\pi (\Gamma_2^0(p, -p))^2 \tilde{\varphi}(p) \tilde{\varphi}(-p) = \int \frac{dp}{2\pi} (p^2 + M^2) \tilde{\varphi}(p) \tilde{\varphi}(-p) \quad (4.25)$$

so if we take the negative root for normalisability of the vacuum functional we get

$$\Gamma_2^0 = -\frac{\sqrt{p^2 + M^2}}{4\pi} \equiv -\frac{\omega(p)}{4\pi}. \quad (4.26)$$

Then it is straightforward to show that

$$\Gamma_2^0 \circ \Gamma_{2n} = - \int dp_1 \dots dp_{2n} \tilde{\varphi}(p_1) \dots \tilde{\varphi}(p_{2n}) \left(\sum_1^{2n} \omega(p_i) \right) \Gamma_{2n}(p_1, \dots, p_{2n}) \delta(p_1 + \dots + p_{2n}) \quad (4.27)$$

which can be used to calculate Γ_4^0 since

$$\Gamma_2^0 \circ \Gamma_4^0 = \frac{g}{4!} \int dx \varphi^4(x) = \frac{g}{4!} \prod_{i=1}^4 \left(\int \frac{dp_i}{2\pi} \tilde{\varphi}(p_i) \right) 2\pi \delta\left(\sum_{j=1}^4 p_j\right) \quad (4.28)$$

and therefore

$$\Gamma_4^0(p_1, \dots, p_4) = -\frac{g}{(2\pi)^3 (4!) (\omega(p_1) + \dots + \omega(p_4))}. \quad (4.29)$$

The terms of higher order in φ , for which there are no contributions from the potential, give, generically,

$$\sum_{n+m=\eta} \Gamma_{2n}^0 \circ \Gamma_{2m}^0 = 0 \quad (4.30)$$

where $\eta \geq 4$ is a constant such that starting with $\eta = 4$ we can determine all the $\Gamma_{2\eta-2}^0$. For example, to determine Γ_6 to leading order we have to solve $\eta = 4$, that is

$$\Gamma_2^0 \circ \Gamma_6^0 + \Gamma_4^0 \circ \Gamma_4^0 + \Gamma_6^0 \circ \Gamma_2^0 = 0. \quad (4.31)$$

and using (4.22) we get

$$\int dp_1 \dots dp_6 \bar{\varphi}(p_1) \dots \bar{\varphi}(p_6) \delta\left(\sum_{i=1}^6 p_i\right) \left(48\pi \Gamma_2^0(-p_1, p_1) \Gamma_6^0(p_1, \dots, p_6) + \right. \\ \left. + 32\pi \Gamma_4^0(-p_1 - p_2 - p_3, p_1, p_2, p_3) \Gamma_4^0(-p_4 - p_5 - p_6, p_4, p_5, p_6) \right) = 0 \quad (4.32)$$

By substituting

$$\Gamma_2^0(-p_1, p_1) \rightarrow \frac{1}{6} \sum_{i=1}^6 \frac{\omega(p_i)}{4\pi} \quad (4.33)$$

in the equation above and using (4.29) we finally get

$$\Gamma_6^0(p_1, \dots, p_6) = \frac{g^2}{(4!)^2 4\pi^5 \sum_{i=1}^6 \omega(p_i)} \mathbf{S} \left\{ \frac{1}{(\omega(p_1 + p_2 + p_3) + \omega(p_1) + \omega(p_2) + \omega(p_3))} \times \right. \\ \left. \times \frac{1}{(\omega(p_4 + p_5 + p_6) + \omega(p_4) + \omega(p_5) + \omega(p_6))} \right\} \quad (4.34)$$

where the \mathbf{S} symmetrises the momenta. The equations (4.30) can be solved recursively as

$$\Gamma_{2r}^0(p_1, \dots, p_{2r}) = \frac{4\pi}{\sum_1^{2r} \omega(p_i)} \sum_{n=2}^{r-1} n(r+1-n) \mathbf{S} \left\{ \Gamma_{2n}^1(-(p_2 + \dots + p_{2n}), p_2, \dots, p_{2n}) \right. \\ \left. \times \Gamma_{2(r+1-n)}^1(-(p_{2n+2} + \dots + p_{2(r+1-n)}), p_{2n+2}, \dots, p_{2(r+1-n)}) \right\} \quad (4.35)$$

If we expand Γ_2^0 and Γ_4^0 in positive powers of the momenta we exactly reproduce (4.3) since no resummation is involved in either approach to the tree level result.

The order \hbar contribution to the Schrödinger equation is

$$\sum_{n,m} \Gamma_{2n}^0 \circ \Gamma_{2m}^{\hbar} + \sum_n \Delta \Gamma_{2n}^0 + \int dx \left(2\mathcal{E}^{\hbar} - (M^2)^{\hbar} \varphi^2(x) \right) = 0. \quad (4.36)$$

Using (4.20) and (4.22) in (4.36) enables us to write the term quadratic in φ as the limit as $\epsilon \rightarrow 0$ of

$$\frac{(\delta M^2 + (M^2(\epsilon))^{\hbar})}{4\pi} + 2\omega(p) \Gamma_2^{\hbar}(p, -p) + \frac{g}{32\pi^2} \int_{q^2 < 1/\epsilon} \frac{dq}{\omega(q) + \omega(p)} = 0 \quad (4.37)$$

which can be solved to give

$$\Gamma_2^{\hbar}(p, -p) = \frac{g}{32\pi^2} \int_0^{\infty} \frac{dq}{(\omega(q) + \omega(p))\omega(q)} - \frac{\delta M^2}{8\pi\omega(p)} \quad (4.38)$$

that is

$$\Gamma_2^{\hbar}(p, -p) = \frac{g}{32\pi^2 p} \operatorname{arcsinh}\left(\frac{p}{M}\right) - \frac{\delta M^2}{8\pi\omega(p)}. \quad (4.39)$$

and for $p = 0$ we get $\Gamma_2^{\hbar} = g/(32\pi^2 M) - \delta M^2/(8\pi M)$. The renormalisation condition that fixes B_2 at its classical value requires that $\Gamma_2^{\hbar}(0, 0) = 0$, which determines

$$\delta M^2 = g/(4\pi), \quad (4.40)$$

but if instead we had chosen a renormalisation condition such that $\delta M^2 = 0$ then we immediately read off the first correction to B_2 ,

$$B_2^{\hbar} = \frac{g}{16\pi}. \quad (4.41)$$

Setting $p = 0$ in (4.37) and taking the limit as $\epsilon \rightarrow 0$ is meant to give the same result as taking the limit $\lambda \rightarrow \infty$ in (4.8) when we identify $\Gamma_2(0, 0) = B_2/(2\pi)$. This gives the value $-g/(8\pi)$ quoted earlier that agrees well with the large λ behaviour of $S(\lambda) - \tilde{M}^2(\lambda)^{\hbar}/2g$. More particularly, $S(\lambda)$ should be obtained from the large ϵ expansion of

$$H(\epsilon) = \frac{1}{16\pi} \int_{q^2 < 1/\epsilon} \frac{dq}{\omega(q) + \omega(p)} \quad (4.42)$$

by applying the two contour integral re-summations, which is formally written as

$$-\frac{\lambda}{4\pi} \int_{|\tilde{s}|=\infty} d\tilde{s} \tilde{s}^{-3/4} e^{\lambda^2 \tilde{s}} \int_{|s|=\infty} ds s^{-1/2} e^{s/\sqrt{\tilde{s}}} H(s) \quad (4.43)$$

which does in fact coincides with (4.9).

Since the large λ behaviour corresponds to small ϵ , we can use (4.39) to investigate this. Thus for small ϵ

$$\begin{aligned} G(\epsilon) &\equiv \int_0^{1/\sqrt{\epsilon}} dq \left(\frac{1}{\omega(q)(\omega(q) + M)} \right) \\ &= \sqrt{M^{-1} + \epsilon} - \sqrt{\epsilon} \approx \sqrt{M} - \sqrt{\epsilon} + \frac{\epsilon}{2\sqrt{M}} - \frac{\epsilon^2}{8\sqrt{M}^3} + \dots \end{aligned} \quad (4.44)$$

which leads to the power law corrections to the large λ behaviour described earlier. The prior knowledge of this small ϵ would have been useful to find an alternative resummation procedure in which we would try to cancel the power law corrections so as to get the exact result given by $\epsilon = 0$. For example, for the small ϵ behaviour described above, the linear combination

$$\left(R(\lambda, \epsilon) + 2R(\lambda, \epsilon)\lambda\epsilon \right) G(\epsilon) \quad (4.45)$$

with $R(\lambda, \epsilon)$ given by (2.23) would subtract the square root correction and increase the convergence. This is because

$$R(\lambda, \epsilon)G(\epsilon) = \sqrt{M} - \frac{1}{\sqrt{\lambda\pi}}\Gamma(1/2) + 0 + 0 + \dots \quad (4.46)$$

whereas

$$2R(\lambda, \epsilon)\lambda\epsilon G(\epsilon) = \frac{1}{\sqrt{\lambda\pi}}\frac{\Gamma(1/2)}{2} + 0 + 0 + \dots \quad (4.47)$$

Expanding (4.39) in positive powers of p^2 leads to the exact results for the W_2^{\hbar} quoted earlier

$$\begin{aligned} & \int \frac{dp}{2\pi} \Gamma_2^{\hbar}(p, -p) \bar{\varphi}(p) \bar{\varphi}(-p) = \\ & -\frac{g}{\pi} \int dx \left(\frac{\varphi'^2}{48} + \frac{3\varphi''^2}{160} + \frac{15\varphi'''^2}{896} + \frac{35\varphi''''^2}{2304} + \frac{315\varphi^{(5)2}}{22528} \right. \\ & \left. + \frac{693\varphi^{(6)2}}{53248} + \frac{1001\varphi^{(7)2}}{81920} + \frac{6435\varphi^{(8)2}}{557056} + \frac{109395\varphi^{(9)2}}{9961472} + \frac{230945\varphi^{(10)2}}{22020096} + \dots \right) \end{aligned} \quad (4.48)$$

The $O(\hbar)$ contribution to the part of $W[\varphi]$ that is quartic in φ is obtained from

$$2\Gamma_2^0 \circ \Gamma_4^{\hbar} + 2\Gamma_4^0 \circ \Gamma_2^{\hbar} + \Delta\Gamma_6^0 = 0. \quad (4.49)$$

Using the equations (4.20) and (4.34), the last term on the left hand side can be expressed as

$$\begin{aligned} \Delta\Gamma_6^0 &= \frac{15g^2}{(4!)^2\pi^4} \int_{q^2 < 1/\epsilon} dq \int dp_1 dp_2 dp_3 dp_4 \bar{\varphi}(p_1) \bar{\varphi}(p_2) \bar{\varphi}(p_3) \bar{\varphi}(p_4) \delta(p_1 + \dots + p_4) \times \\ & \frac{1}{(2\omega(q) + \sum_1^4 \omega(p_i))} \mathbf{S} \left\{ \frac{2/5}{(2\omega(q) + 2\omega(p_1))(\omega(p_2 + p_3 + p_4) + \omega(p_2) + \omega(p_3) + \omega(p_4))} + \right. \\ & \left. \frac{3/5}{(\omega(p_1 + p_2 - q) + \omega(q) + \omega(p_1) + \omega(p_2))(\omega(q + p_3 + p_4) + \omega(q) + \omega(p_3) + \omega(p_4))} \right\} \end{aligned} \quad (4.50)$$

which together with (4.27) and (4.29), enable us to solve (4.49) for Γ_4^{\hbar} to give

$$\begin{aligned} \Gamma_4^{\hbar}(p_1, \dots, p_4) &= \frac{g^2}{(2\pi)^3 4! \pi \sum_1^4 \omega(p_i)} \mathbf{S} \left\{ \int_0^\infty \frac{dq}{2\omega(q) + \sum_1^4 \omega(p_i)} \left(-\frac{1}{2\omega(q)(\omega(q) + \omega(p_1))} \right. \right. \\ & \left. \left. + \frac{3}{(\omega(q) + \omega(p_1) + \omega(p_2) + \omega(q + p_1 + p_2))(\omega(q) + \omega(p_3) + \omega(p_4) + \omega(-q + p_3 + p_4))} \right) \right. \\ & \left. + \frac{1}{2\omega(p_1) \sum_1^4 \omega(p_i)} \right\} \end{aligned} \quad (4.51)$$

Notice that this expression has to be symmetrised in the momenta, which has been symbolised by \mathbf{S} . For instance, if we write the second term in the parenthesis as $F(p_1, p_2, p_3, p_4)$ then

$$\begin{aligned} \mathbf{S} F(p_1, p_2, p_3, p_4) &= \frac{1}{6} \left(F(p_1, p_2, p_3, p_4) + F(p_3, p_4, p_1, p_2) + F(p_1, p_3, p_2, p_4) \right. \\ &\quad \left. + F(p_2, p_4, p_1, p_3) + F(p_1, p_4, p_2, p_3) + F(p_2, p_3, p_1, p_4) \right), \end{aligned} \quad (4.52)$$

and that the last term in the curly brackets originates from the δM^2 term in (4.39).

Expanding (4.51) in powers of the momenta and integrating over q numerically enable us to write an exact expression for the first order corrections to the four field basis functions, that is

$$\begin{aligned} W_4^{\hbar} &= \frac{g^2}{10000} \int dx \left(3.973\varphi^4 - 19.45\varphi^2\varphi'^2 - 7.961\varphi'^4 \right. \\ &\quad \left. + 16.27\varphi^2\varphi''^2 + 85.78\varphi'^2\varphi''^2 + 33.66\varphi\varphi'^3 - 14.15\varphi^2\varphi'''^2 \right. \\ &\quad \left. + 12.65\varphi^2\varphi''''^2 + 84.76\varphi''^4 - 150.7\varphi\varphi''\varphi''''^2 - 139.0\varphi'^2\varphi''''^2 + \dots \right). \end{aligned} \quad (4.53)$$

From this it is clear that our previous estimate was quite good, but that the observation that the ratios

$$\rho_{j_0, \dots, j_n} = \frac{B_{j_0, \dots, j_n}^{\hbar}}{g B_{j_0, \dots, j_n}^0} \quad (4.54)$$

are the same for coefficients of functionals of the same dimension and number of fields is only approximate since

$$\rho_4 = -0.03814 \quad (4.55)$$

$$\rho_{2,2} = -0.1245 \quad (4.56)$$

$$\rho_{0,4} = -0.2038, \rho_{2,0,2} = -0.2082 \quad (4.57)$$

$$\rho_{0,2,2} = -0.2834, \rho_{1,0,3} = -0.2872, \rho_{2,0,0,2} = -0.2898 \quad (4.58)$$

$$\rho_{2,0,0,0,2} = -0.3701, \rho_{0,0,4} = -0.3734, \rho_{1,0,1,2} = -0.3769, \rho_{0,2,0,2} = -0.3799. \quad (4.59)$$

These ratios can, however, be explained by observing that the dominant contribution to (4.51) comes from the term originated in the mass renormalisation prescription, $\hbar\delta M^2$, which was fixed by imposing $B_2^{\hbar} = 0$. If instead we had chosen our renormalisation conditions $\hbar\delta M^2 = 0$ then it would have been absent in that expression.

We can easily calculate the effect of this choice on the ratios using dimensional analysis. The coefficient of a basis function of dimension D , i.e. with a total of D derivatives, reads, in terms of the dimensionful parameters of the theory,

$$B_D = B_D^0 \frac{g}{M^{D+1}} + B_D^\hbar \frac{g^2}{M^{D+3}} + \dots, \quad (4.60)$$

where B_D^0 and B_D^\hbar are dimensionless constants. Hence

$$\delta B_D = -\frac{B_D^0 g (D+1) \delta M^2}{2} + O(\hbar^2), \quad (4.61)$$

having chosen our mass scale such that $M = 1$, which allows us to write the ratio ρ as

$$\rho_D = \frac{B_D^\hbar}{g B_D^0} - \frac{(D+1) \delta M^2}{2} = \bar{\rho}_D - \frac{D+1}{8\pi} \quad (4.62)$$

where in the last equality $\bar{\rho}$ is the ratio for the renormalisation condition $\delta M^2 = 0$. Thus

$$\bar{\rho}_4 = -0.00165 \quad (4.63)$$

$$\bar{\rho}_{2,2} = -0.00513 \quad (4.64)$$

$$\bar{\rho}_{0,4} = -0.00486, \quad \bar{\rho}_{2,0,2} = -0.00926 \quad (4.65)$$

$$\bar{\rho}_{0,2,2} = -0.00488, \quad \bar{\rho}_{1,0,3} = -0.00868, \quad \bar{\rho}_{2,0,0,2} = -0.0113 \quad (4.66)$$

$$\bar{\rho}_{2,0,0,0,2} = -0.0120, \quad \bar{\rho}_{0,2,0,2} = -0.0220, \quad \bar{\rho}_{1,0,1,2} = -0.0188, \quad \bar{\rho}_{0,0,4} = -0.0153. \quad (4.67)$$

The advantage of this choice is that the one-loop corrections to the coefficients B_{j_0, \dots, j_n} for functionals containing four fields are now significantly smaller. The same is true for the coefficients corresponding to two fields, with the exception of B_2 . This suggests that a more effective choice of renormalisation condition which would reduce the size of the one-loop corrections, would be to fix B_4 at its classical value, rather than B_2 [4].

4.6 Sinh-Gordon Model

From the standpoint of perturbation theory φ^4 -theory is 'close' to a theory that is quite special, namely the Sinh-Gordon theory which has an infinite number of conserved quantities that imply the absence of particle production, it is interesting to calculate the vacuum functional for this case. The potential of the Sinh-Gordon theory may be taken to be [45]

$$V = \frac{M^2 + \hbar \delta M^2}{\beta^2} \cosh(\beta \phi) \exp \left(-\frac{\beta^2}{4\pi} \int_0^{1/\sqrt{\epsilon}} \frac{dp}{\omega(p)} \right) = \\ (M^2 + \hbar \delta M^2) \left(\frac{1}{\beta^2} + \frac{\phi^2}{2} + \frac{\beta^2 \phi^4}{4!} + \frac{\beta^4 \phi^6}{6!} + \dots \right) \left(1 - \frac{\beta^2}{4\pi} \int_0^{1/\sqrt{\epsilon}} \frac{dp}{\omega(p)} + \dots \right) \quad (4.68)$$

Apart from the replacement $g \rightarrow M^2\beta^2$ the Sinh-Gordon potential leads to the same expressions for the tree-level values of Γ_2^1, Γ_4^1 and the one-loop result Γ_2^{\hbar} . The tree-level Γ_6^1 is modified by the ϕ^6 term in the potential

$$\Gamma_6^1 \rightarrow \Gamma_6^1 - \frac{\beta^4 M^2}{6!(2\pi)^5 \sum_1^6 \omega(p_i)} \quad (4.69)$$

this, together with the $\delta M^2 \phi^4$ term in V modifies the one-loop value Γ_4^{\hbar}

$$\Gamma_4^{\hbar} \rightarrow \Gamma_4^{\hbar} - \frac{\beta^4 M^2}{(2\pi)^4 4! \sum_1^4 \omega(p_i)} \left(\int_0^\infty dq \left(\frac{1}{2\omega(q) + \sum_1^4 \omega(p_i)} - \frac{1}{2\omega(q)} \right) + \frac{1}{2} \right) \quad (4.70)$$

so that for the sinh-Gordon model

$$\begin{aligned} W_4^{\hbar} &= \frac{\beta^4}{\pi} \int dx \left(\frac{\phi^4}{384} + \frac{5\pi - 22}{1280} \phi^2 \phi'^2 - \frac{2275\pi - 8952}{860160} \phi'^4 + \frac{651\pi - 2768}{172032} \phi^2 \phi''^2 \right. \\ &\quad - \frac{1041705\pi - 4243072}{41287680} \phi'^2 \phi''^2 - \frac{689535\pi - 2920448}{82575360} \phi \phi''^3 \\ &\quad \left. + \frac{13905\pi - 58624}{3932160} \phi^2 \phi'''^2 + \dots \right) \\ &\simeq \frac{\beta^4}{10000} \int dx \left(8.2893\phi^4 - 15.647\phi^2 \phi'^2 - 6.6791\phi'^4 \right. \\ &\quad \left. + 13.3743\phi^2 \phi''^2 + 74.818\phi'^2 \phi''^2 + 29.0731\phi \phi''^3 - 12.0941\phi^2 \phi'''^2 + \dots \right). \quad (4.71) \end{aligned}$$

The ratios of the one-loop coefficients to their tree-level values for this model are

$$\rho_4 = -0.07958 \quad (4.72)$$

$$\rho_{2,2} = -0.1001 \quad (4.73)$$

$$\rho_{0,4} = -0.1710, \quad \rho_{2,0,2} = -0.1712 \quad (4.74)$$

$$\rho_{0,2,2} = -0.2471, \quad \rho_{1,0,3} = -0.2481, \quad \rho_{2,0,0,2} = -0.2477. \quad (4.75)$$

Note that again the ratios are approximately the same for coefficients of functionals of the same number of fields and dimension, however this cannot be explained away as simply the effect of mass or coupling renormalisation. If we had taken $\delta M^2 = 0$ we would have obtained ³

$$\rho_4 = -0.1194 \quad (4.76)$$

$$\rho_{2,2} = -0.06035 \quad (4.77)$$

$$\rho_{0,4} = -0.05162, \quad \rho_{2,0,2} = -0.05183 \quad (4.78)$$

³For this model, equation (4.62) becomes $\rho_D = \bar{\rho}_D - (D-1)/(8\pi)$.

$$\rho_{0,2,2} = -0.04820, \quad \rho_{1,0,3} = -0.04915, \quad \rho_{2,0,2} = -0.04875. \quad (4.79)$$

which are approximately constant for coefficients of functionals of the same number of fields and dimension. These coefficients would, with a change of sign, apply to the Sine-Gordon model as well.

4.7 Reconstructing the Vacuum Functional

We finish this chapter by illustrating how we can reconstruct the vacuum functional from its large distance expansion, as we discussed in section 2.3, using some of the results we derived in this chapter.

Let us concentrate on the quadratic part of the logarithm of the vacuum functional,

$$\int dp \varphi(p) \varphi(-p) \Gamma(p, -p) \quad (4.80)$$

Applying the formula (2.34) in the expression above, is equivalent to writing

$$\Gamma_2(p, -p) = \lim_{\lambda \rightarrow \infty} \frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s-1} e^{\lambda(s-1)} \sqrt{s} \Gamma_2(p/\sqrt{s}, -p/\sqrt{s}) \quad (4.81)$$

Since $|s|$ is large on the contour we can use the local expansion $\Gamma_2(p, -p) = \sum_0^\infty a_n p^{2n}$.

Shifting s we get

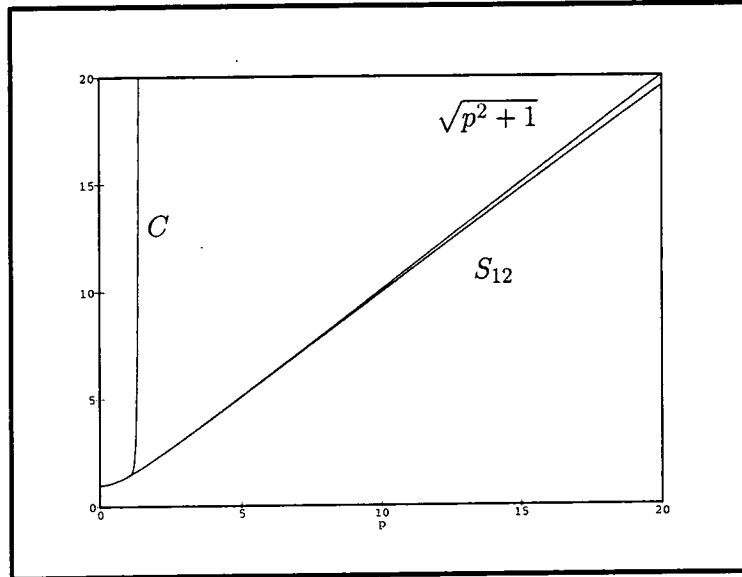
$$\lim_{\lambda \rightarrow \infty} \frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s} e^{\lambda s} \sqrt{s+1} \sum_0^\infty a_n \frac{p^{2n}}{(s+1)^n} \equiv \lim_{\lambda \rightarrow \infty} S(p, \lambda) \quad (4.82)$$

Expanding the $(s+1)$ factors in powers of $1/s$ enables the integral to be done, yielding a power series in λ . For example, at tree-level

$$\frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s-1} e^{\lambda(s-1)} \sqrt{p^2 + s} = \sum_0^\infty \frac{(-)^{n+1} \lambda^{n-1/2} (1+p^2)^n}{n!(2n-1)\sqrt{\pi}}. \quad (4.83)$$

This series converges for all positive λ . We get an approximation by truncating the expansion by including terms up to and including $\lambda^{N-1/2}$, say. This requires a knowledge of the local expansion only up to terms in $(\varphi^{(N)}(x))^2$. To demonstrate this approximation we have plotted in fig. (4.5) the series (4.83) truncated at $N = 12$, S_{12} .

The value of λ is chosen so that the last term included is one per cent of the value of the series. We have also plotted $\sqrt{p^2 + 1}$, and the expansion of $\sqrt{p^2 + 1}$ in powers of p^2 , C truncated to fourteen terms. The full series fails to converge for $p^2 > 1$, and this is reflected in the fact that the truncated series ceases to be a good approximation for

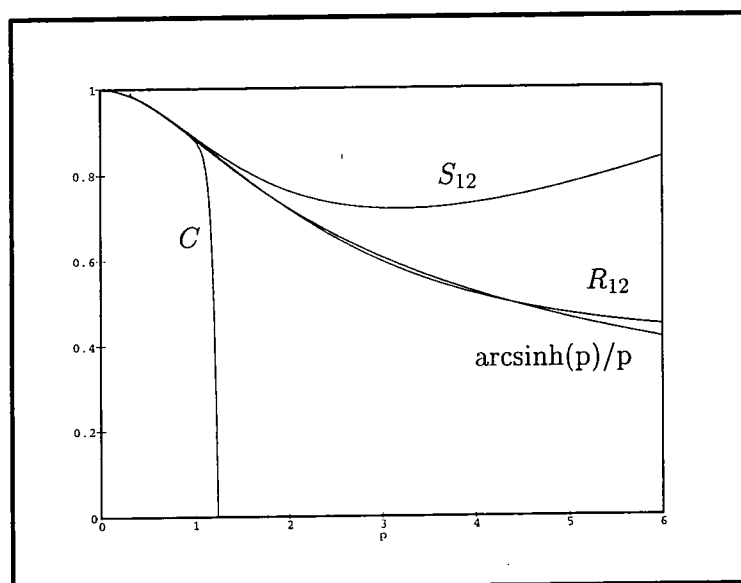
Figure 4.5: Tree-level vacuum functional: $\Gamma_2^1(p, -p)$

$p^2 > 1$. However, S_{12} , which is a resummation of this series is a very good approximation for a much larger range of momenta.

The one-loop correction, Γ_2^{\hbar} , may be treated in the same way. In fig. (4.6) we have plotted $\text{arcsinh}(p)/p$. The small p expansion, C is again only good for $p^2 < 1$. Our approximation that re-sums this series, S_{12} provides a good approximation only over a slightly larger range. The accuracy of this approximation is greatly improved by further re-summations, just as we did for the Laplacian. Let us define the resummation operator acting on a function of λ and p to be

$$R \cdot S(\lambda, p) \equiv \frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s} e^{\lambda s} S(s^{-1/2}, p). \quad (4.84)$$

Then the curve R_{12} shown in fig. (4.6) results from applying R twice to S_{12} , and provides a good approximation to $\text{arcsinh}(p)/p$ for values of p up to about $p = 5$. Since the effect of applying R^p to a term in S_{12} that is proportional to λ^n is simply to divide it by $\Gamma(n/2 + 1)\Gamma(n/4 + 1) \dots \Gamma(n/2^p + 1)$ further applications would have no significant effect when we take just twelve terms in the expansion.

Figure 4.6: One-loop vacuum functional: $\Gamma_2^k(p, -p)$

Chapter 5

Feynman Diagram Expansion of the ϕ_{1+1}^4 Vacuum Functional

Representing the vacuum functional as a functional integral enables us to derive its semi-classical solution within the conventional approach to quantum field theory based on the language of Feynman diagrams. The advantage of this formalism is obviously the gain of pictorial insight as well as the possibility of associating simple general rules to the diagrams and therefore reduce the problem to the calculation of integrals over the space-time.

5.1 Introduction

In section 2.2, we obtained a functional integral representation for the vacuum functional of a scalar theory from the Feynman path integral representation of the Schrödinger functional. Let us recall that expression here:

$$\Psi[\varphi] = e^{W[\varphi]} = \int \mathcal{D}\phi e^{-S_E[\phi] + \int dx \dot{\phi}(x,0)\varphi(x)} \equiv \int \mathcal{D}\phi e^{-S_E + S_B} \quad (5.1)$$

The Euclidean action $S_E[\phi]$ is defined on the half plane $t \leq 0$ where the field ϕ satisfies boundary condition $\phi(x, 0) = 0$. The logarithm of the vacuum functional $W[\varphi]$ can be seen as a sum of connected Feynman diagrams in which φ is the source for $\dot{\phi}$ on the boundary, where ϕ vanishes.

A stationary phase approximation to (5.1) reproduces the semi-classical, \hbar -expansion. Hence we can formally write

$$W[\varphi] = -S_E[\varphi_{class}] - \ln(\text{Det}\Lambda_0) - \dots \quad (5.2)$$

where φ_{class} is the on-shell classical field evolving from a fixed value, say zero, in the

infinite Euclidean past, to the value φ at $t = 0$. Λ_0 stands for the second derivative of S_E evaluated for the classical field and the dots represent multi-loop terms. From this the resemblance to the well-known effective action description of quantum field theory is clear. The novelty in our description of the vacuum functional is the presence of the boundary, where the field satisfies Dirichlet boundary conditions and has a source term S_B .

In this chapter, we develop a Feynman diagram picture of the ϕ_{1+1}^4 theory vacuum functional, which can be suitably extended to Sine-Gordon models. In this approach, we reproduce some of the results which were obtained from the (exact) semi-classical solution of the Schrödinger equation in chapter 4. We also rely on Symanzik's work which establishes the finiteness of the wave functional as any cut-off is removed. For ϕ^4 theory in two dimensions, no additional field renormalisation associated with possible new divergences due to the boundary is necessary, although it is in $(3 + 1)$ dimensions. Thus we should only face the usual renormalisation procedure which involves the divergences that occur in the bulk of the space-time. For any scalar theory in two dimensions with no derivative interactions this is rather simple: the only ultra-violet diagrams that occur in any order of perturbation theory comprise the graphs that contain a closed loop consisting of a single internal line, that is, two fields at the same vertex contracted with each other [45]. In this case, the ultra-violet divergence can be removed by normal-ordering the Hamiltonian as we have seen for ϕ_{1+1}^4 theory. As a matter of illustration, we show in fig.5.1 two loop diagrams for ϕ_{1+1}^4 theory. The diagram (a) is ultra-violet divergent whereas (b) is finite.

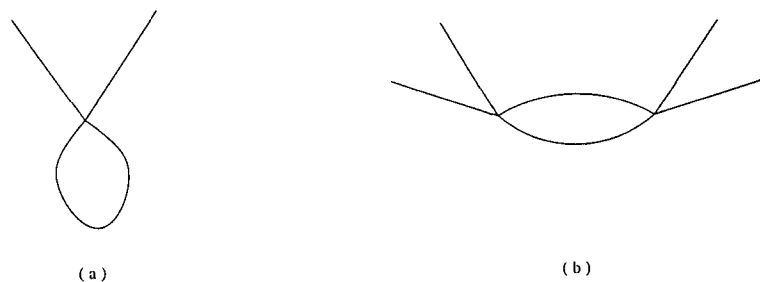


Figure 5.1: Diagram (a) is UV divergent. Diagram (b) is convergent

5.2 Feynman Diagrams on the Boundary

Let us start by establishing our notation. As we will be working in two dimensions throughout this chapter, let us take the vertical direction as the time-like direction and the horizontal direction as the space-like direction. Therefore $P = (t, x)$ is any point in the Euclidean half-plane with t in the range $-\infty \leq t \leq 0$ and $-\infty \leq x \leq \infty$, $t = 0$ being the equation which defines the boundary.

In constructing the Feynman diagram expansion of $W[\varphi]$, the only major difference from the usual Feynman diagrams encountered in free space is that the propagator vanishes when either of its arguments lies on the boundary. Such a propagator can be constructed using the method of images as

$$G_D(x, y) \equiv G_0(x, y) - G_0(\underline{x}, y) = G_0(x, y) - G_0(x, \underline{y}) \quad (5.3)$$

where $x = (t, \mathbf{x})$, $\underline{x} = (-t, \mathbf{x})$ and G_0 is the free space propagator. Notice that on the boundary $t = 0$, G_D , which we henceforth call Dirichlet propagator, vanishes. Furthermore, because of the breaking of translation symmetry in the time-like direction, we may have non-conservation of the momentum component in this direction. In other words, the boundary might affect the “energy” conservation.

We write the Euclidean action for ϕ_{1+1}^4 theory on the half-plane as

$$S_E[\phi] = \int_{t < 0} dt \int dx \left(\frac{1}{2} \dot{\phi}^2 + \frac{1}{2} \phi'^2 + \frac{1}{2} M^2(s) \phi^2 + \frac{g}{4!} \phi^4 \right) \quad (5.4)$$

and since only mass renormalisation is required because of the divergent tadpoles, we cut-off the momentum integration with $1/s$ in

$$M^2(s) = M^2 - \frac{g}{2} \int_{p^2 < 1/s} \frac{d^2 p}{(2\pi)^2} \frac{1}{p^2 + M^2} \quad (5.5)$$

$p^2 + M^2 = E^2 + \mathbf{p}^2 + M^2$. We make connection with equation (3.11) by performing one of the integrals over the momenta to yield (3.11) with $\delta M^2 = 0$.

The source term is

$$S_B = \int d\mathbf{x} \varphi(\mathbf{x}) \dot{\phi}(0, \mathbf{x}) = \int d\mathbf{x} dt \varphi(\mathbf{x}) \dot{\phi}(t, \mathbf{x}) \delta(t) \quad (5.6)$$

which fourier-analysed using

$$\begin{aligned} \varphi(\mathbf{x}) &= \int \frac{d\mathbf{p}}{2\pi} e^{i\mathbf{p} \cdot \mathbf{x}} \tilde{\varphi}(\mathbf{p}) \\ \phi(x) &= \int \frac{d^2 p}{(2\pi)^2} e^{ipx} \tilde{\phi}(p) \end{aligned} \quad (5.7)$$

gives

$$S_B = \int \frac{dE_p d\mathbf{p}}{(2\pi)^2} iE_p \tilde{\varphi}(-\mathbf{p}) \tilde{\phi}(E, \mathbf{p}). \quad (5.8)$$

From this we see that, in momentum space, a factor of iE_p accompanies the source $\tilde{\varphi}(-\mathbf{p})$.

Likewise, we fourier-transform the Green's function

$$\begin{aligned} \int d^2x d^2y e^{-i(px+qy)} G_0(x, y) &= \int d^2x d^2y e^{-i(px+qy)} \int \frac{d^2k}{(2\pi)^2} \frac{e^{ik(x-y)}}{k^2 + M^2} \\ &= \frac{1}{p^2 + M^2} \delta^2(p + q) \end{aligned} \quad (5.9)$$

for the free space propagator and

$$\int d^2x d^2y e^{-i(px+qy)} G_0(\underline{x}, y) = \frac{\delta(\mathbf{p} + \mathbf{q}) \delta(E_p - E_q)}{(p^2 + M^2)} \quad (5.10)$$

for the image propagator. We graphically represent the Dirichlet propagator shown in fig.5.2 as a sum of the free space propagator (full line) and the image, energy non-conserving propagator (dashed line).

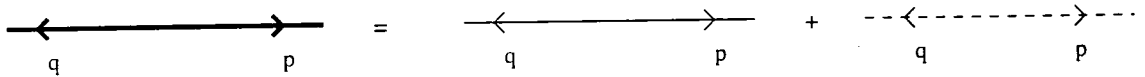


Figure 5.2: Dirichlet Propagator

We can start writing the Feynman rules in the momentum space for the Feynman diagram expansion of the ϕ_{1+1}^4 theory vacuum functional. $W[\varphi]$ is a collection of connected Feynman diagrams with the “legs” attached to the boundary for which

- at each interaction point \times we associate a factor g (coupling constant);
- at each source field placed on the boundary, we write $\int \frac{d^2p}{(2\pi)^2} \tilde{\varphi}(-\mathbf{p}) iE_p$
- a propagator is composed by two pieces, as shown in fig.5.2. For each propagator we associate a factor $\frac{1}{p^2 + M^2} \left(\delta^2(p + q) + \delta(\mathbf{p} + \mathbf{q}) \delta(E_p - E_q) \right)$;
- The mass counterterm is given by (5.5);
- A symmetry factor s_f is to be associated to a diagram. It comprises the product of three different numbers: the expansion factor of the exponential in (5.1), the different ways of contracting the source fields with the vertices (which reflects how well the factors of $1/4!$ in $g/4!$ have been canceled at each vertex) and the number of topologically distinct diagrams.

When the diagram involves loops, the Feynman rules in the momentum space are not as straightforward as they are in the free space. Let us work out a few examples. Consider the simplest graph in the diagrammatic expansion of $W[\varphi]$, shown in fig.5.3(a)



Figure 5.3: (a) Tree-level two-field diagram

For this diagram, we can use our Feynman rules to write

$$-s_f \int_{pq} \tilde{\varphi}(-\mathbf{p}) \tilde{\varphi}(-\mathbf{q}) E_p E_q \frac{1}{p^2 + M^2} \left(\delta^2(p+q) + \delta(\mathbf{p}+\mathbf{q}) \delta(E_p - E_q) \right) \quad (5.11)$$

$$= 2 s_f \int_p \tilde{\varphi}(\mathbf{p}) \tilde{\varphi}(-\mathbf{p}) \frac{(E_p)^2}{E_p^2 + \mathbf{p}^2 + M^2}. \quad (5.12)$$

where we adopt the following convention

$$\begin{aligned} \int_p &\sim \int_{E_p} \int_{\mathbf{p}} \sim \int_{-\infty}^{\infty} \frac{dE_p}{2\pi} \int_{-\infty}^{\infty} \frac{d\mathbf{p}}{2\pi} \\ \int_x &\sim \int_t \int_{\mathbf{x}} \sim \int_{-\infty}^0 dt \int_{-\infty}^{\infty} d\mathbf{x} \end{aligned} \quad (5.13)$$

First of all, we learn from this simple example that when a propagator ends on the boundary it equals two times the free space propagator, viz.

$$\int_p \tilde{\varphi}(-\mathbf{p}) iE_p \frac{1}{p^2 + M^2} \left(\delta^2(p+q) - \delta(\mathbf{p}+\mathbf{q}) \delta(E_p - E_q) \right) = 2 \left(\frac{-1}{(2\pi)^2} \frac{\tilde{\varphi}(\mathbf{q}) iE_q}{q^2 + M^2} \right), \quad (5.14)$$

which is schematically represented in fig.5.4

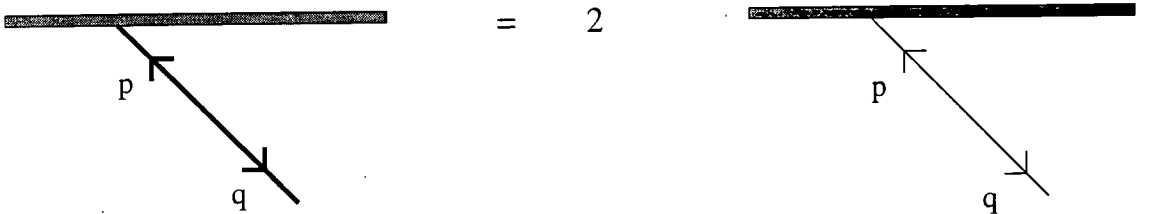


Figure 5.4:

Notice, however, that the E_p integral in (5.12) is not convergent. It can formally be written as

$$\int_{-\infty}^{\infty} \frac{dE_p}{(2\pi)} \left(\frac{E_p^2}{E_p^2 + \mathbf{p}^2 + M^2} \right) \equiv \int_{-\infty}^{\infty} \frac{dE_p}{(2\pi)} \left(1 - \frac{\mathbf{p}^2 + M^2}{E_p^2 + \mathbf{p}^2 + M^2} \right)$$

$$= \delta(0) - \frac{\sqrt{\mathbf{p}^2 + M^2}}{2} \quad (5.15)$$

The origin of $\delta(0)$ is in the construction of our path integral representation of W (please see section 2.2). We started by representing the vacuum functional as the matrix element

$$\Psi[\varphi] = \langle \varphi | 0 \rangle = \langle D | e^{i \int \hat{\pi} \varphi dx} | 0 \rangle \quad (5.16)$$

As operators, $\hat{\pi} = \dot{\hat{\phi}}$, but in the passage from (5.16) to a functional integral representation, which is written in terms of c -numbers, $\hat{\pi}$ is represented by $\dot{\phi}$ plus terms coming from the time derivative acting on the T -ordering, because the functional integral represents T -ordered products:

$$T(\hat{\pi}(\mathbf{x}, t) \hat{\pi}(\mathbf{x}', t')) = \frac{\partial^2}{\partial t \partial t'} T(\hat{\phi}(\mathbf{x}, t) \hat{\phi}(\mathbf{x}', t')) - i \delta(\mathbf{x} - \mathbf{x}') \delta(t - t') \quad (5.17)$$

(in Minkowski space) [55]. This leads to a term like

$$\int d\mathbf{x} d\mathbf{x}' \varphi(\mathbf{x}) \varphi(\mathbf{x}') \delta(\mathbf{x} - \mathbf{x}') \delta(0 - 0) \quad (5.18)$$

but because this is local, it may be canceled by an equal and opposite counterterm, $-\int d\mathbf{x} \Lambda \varphi^2(\mathbf{x})$ say, which amounts to simply discarding this divergence [2]. Alternatively, and perhaps more satisfactorily, we can place the source term not at $t = 0$, but at small, distinct times t_i , and finally taking the limit $t_i \rightarrow 0$. This replaces the integral in (5.15) by

$$\int_{-\infty}^{\infty} \frac{dE_p}{(2\pi)} \frac{E_p^2}{E_p^2 + \mathbf{p}^2 + M^2} e^{iE_p \epsilon}. \quad (5.19)$$

The factor $e^{iE_p \epsilon}$ regularises the divergence and in the complex E_p -plane, for $\epsilon > 0$ we can close the contour integral in the upper half plane to get the result $-\sqrt{\mathbf{p}^2 + M^2}/2$. Hence, the diagram represented in fig.5.3(a) corresponds to the expression

$$-\frac{1}{4\pi} \int d\mathbf{p} \tilde{\varphi}(\mathbf{p}) \tilde{\varphi}(-\mathbf{p}) \sqrt{\mathbf{p}^2 + M^2} \quad (5.20)$$

where $s_f = 1/2$, which reproduces Γ_2^0 obtained in chapter 4 as we expected.

The Feynman rules in the coordinate space for the diagram in fig.5.3(a) give

$$s_f \int d\mathbf{x}_1 d\mathbf{x}_2 \varphi(\mathbf{x}_1) \varphi(\mathbf{x}_2) \left. \frac{\partial G_D(x_1, x_2)}{\partial t_1 \partial t_2} \right|_{t_1=0, t_2=0} \quad (5.21)$$

since the normal (time) differentiation bends the leg of the propagator to the boundary. The property that when one end of the Dirichlet propagator is on the boundary it equals twice the free space propagator is easily seen in the coordinate space since

$$\frac{\partial G_D(x_1, x_2)}{\partial t_1} = 2 \frac{\partial G_0(x_1, x_2)}{\partial t_1} \quad (5.22)$$

Using (5.9) and that

$$\left. \frac{\partial G_D(x_1, x_2)}{\partial t_1 \partial t_2} \right|_{t_1=t_2=0} = \int_p 2E_p^2 \frac{e^{i\mathbf{p}\cdot(\mathbf{x}_1-\mathbf{x}_2)}}{p^2 + M^2}, \quad (5.23)$$

(5.21) becomes

$$s_f \int d\mathbf{x}_1 d\mathbf{x}_2 \varphi(\mathbf{x}_1) \varphi(\mathbf{x}_2) \int_p 2E_p^2 \frac{e^{i\mathbf{p}\cdot(\mathbf{x}_1-\mathbf{x}_2)}}{p^2 + M^2} \quad (5.24)$$

which reduces to (5.12) after integrating over the coordinates. Acting on (5.24) with the laplacian

$$\Delta_s = \int d\mathbf{x}' d\mathbf{y}' \int_{q^2 < 1/s} \frac{d\mathbf{q}}{(2\pi)} e^{i\mathbf{q}\cdot(\mathbf{x}'-\mathbf{y}')} \frac{\delta^2}{\delta\varphi(\mathbf{x}')\delta\varphi(\mathbf{y}')} \quad (5.25)$$

gives the negative of the $O(\hbar)$ vacuum energy density. The action of the functional derivatives in the laplacian has the effect of coalescing the legs of the diagram shown in fig.5.3(a), so to speak, to produce the bubble shown in fig.5.3(b) .

5.3 Tree Level Feynman Diagrams

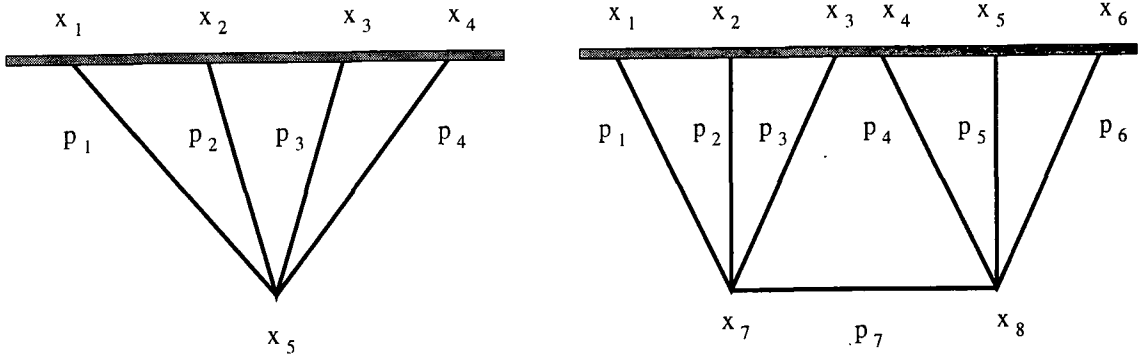


Figure 5.5: Tree Level Diagrams up to φ^6

The Feynman rules in the coordinate space applied to the first diagram in fig.5.5 yield

$$16gs_f \int_{\mathbf{x}_1 \mathbf{x}_2 \mathbf{x}_3 \mathbf{x}_4 \mathbf{x}_5} \varphi(\mathbf{x}_1) \varphi(\mathbf{x}_2) \varphi(\mathbf{x}_3) \varphi(\mathbf{x}_4) \frac{\partial G_0(x_1, x_5)}{\partial t_1} \frac{\partial G_0(x_2, x_5)}{\partial t_2} \frac{\partial G_0(x_3, x_5)}{\partial t_3} \frac{\partial G_0(x_4, x_5)}{\partial t_4} \quad (5.26)$$

where the normal derivatives are always calculated at $t_i = 0$. Using that

$$\left. \frac{\partial G_0(x_1, x_5)}{\partial t_5} \right|_{t_5=0} = \int_{p_1} iE_1 \frac{e^{i(x_1-x_5)p_1}}{p_1^2 + M^2} \quad (5.27)$$

etc., and writing the fields in the momentum space, enables us to write (5.26) as

$$16gs_f \int_{p_1 p_2 p_3 p_4 x_5} \tilde{\varphi}(\mathbf{p}_1) \tilde{\varphi}(\mathbf{p}_2) \tilde{\varphi}(\mathbf{p}_3) \tilde{\varphi}(\mathbf{p}_4) E_1 E_2 E_3 E_4 \times$$

$$\frac{e^{-i(E_1+E_2+E_3+E_4)t_5} e^{-i(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3+\mathbf{p}_4)\mathbf{x}_5}}{\prod_{j=1}^4 (p_j^2 + M^2)} \quad (5.28)$$

The integrals over t_5 and \mathbf{x}_5 can be calculated to yield delta functions in the momenta.

However, notice that the t_5 integration runs from $-\infty$ to 0 :

$$\int_{-\infty}^0 dt_5 e^{-i(E_1+E_2+E_3+E_4)t_5} = \int_0^{\infty} dt_5 e^{i(E_1+E_2+E_3+E_4)t_5} = \int_0^{\infty} dt_5 e^{-i(E_1+E_2+E_3+E_4)t_5} \quad (5.29)$$

where in the first equality we changed variables $t_5 \rightarrow -t_5$ and in the second, we used that $E_1, E_2, E_3, E_4 \rightarrow -E_1, -E_2, -E_3, -E_4$ is a symmetry of (5.28). Hence

$$\int_{-\infty}^0 dt_5 e^{-i(E_1+E_2+E_3+E_4)t_5} = \frac{2\pi}{2} \delta(E_1 + E_2 + E_3 + E_4) \quad (5.30)$$

and (5.28) becomes

$$16g_s f \frac{(2\pi)^2}{2} \int_{p_1 p_2 p_3 p_4} \tilde{\varphi}(\mathbf{p}_1) \tilde{\varphi}(\mathbf{p}_2) \tilde{\varphi}(\mathbf{p}_3) \tilde{\varphi}(\mathbf{p}_4) E_1 E_2 E_3 E_4 \frac{\delta^2(\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3 + \mathbf{p}_4)}{\prod_{j=1}^4 (p_j^2 + M^2)} \quad (5.31)$$

The integrals over $E_1 \dots E_5$ are readily computed in the complex E_i -plane, using the residue's theorem,

$$\int_{-\infty}^{\infty} \frac{d\alpha}{2\pi} \left\{ \prod_{j=1}^4 \left(\int \frac{dE_j}{2\pi} \frac{E_j e^{i\alpha E_j}}{(E_j^2 + \omega_j^2)} \right) \right\} = \frac{1}{16\pi \sum_{j=1}^4 \omega_j} \quad (5.32)$$

with $\omega_j^2 = \mathbf{p}_j^2 + M^2$. Using these results in (5.31), with $s_f = -1/4!$ is just Γ_4^0 obtained in chapter 4.

The action of the laplacian (5.25) on the tree-level, four-legged diagram reads

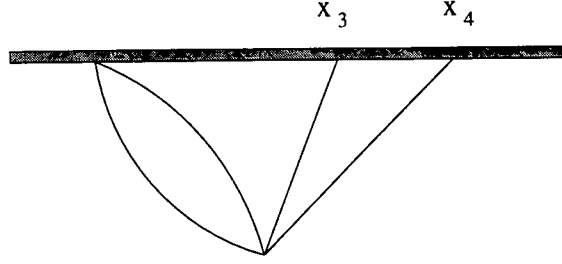
$$\Delta_s \left(\frac{-g}{(2\pi)^3 4!} \int d\mathbf{p}_1 \dots d\mathbf{p}_4 \int_{\mathbf{x}_1 \dots \mathbf{x}_4} \varphi(\mathbf{x}_1) \dots \varphi(\mathbf{x}_4) e^{i(\mathbf{p}_1 \mathbf{x}_1 + \dots + \mathbf{p}_4 \mathbf{x}_4)} \frac{\delta(\mathbf{p}_1 + \dots + \mathbf{p}_4)}{\sum_{j=1}^4 \omega_j} \right) \quad (5.33)$$

and results

$$12 \frac{-g}{2^4 3} \int_{q^2 < 1/s} \int_{\mathbf{p}_3 \mathbf{x}_3 \mathbf{x}_4} \varphi(\mathbf{x}_3) \varphi(\mathbf{x}_4) \frac{e^{i\mathbf{p}_3(\mathbf{x}_3 - \mathbf{x}_4)}}{\omega_q + \omega_3}. \quad (5.34)$$

The factor 12 is the number of possibilities of acting the two functinal derivatives on the four fields. This expression corresponds to the term $\Delta\Gamma_4^0$ in (4.37) and is graphically represented in fig.5.6. Expanding in powers of the momenta amounts to expanding $\varphi(\mathbf{x}_4)$ around \mathbf{x}_3 , that is

$$\frac{-g}{4} \sum_n \int_{q^2 < 1/s} \int_{\mathbf{p}_3 \mathbf{x}_3 \mathbf{x}_4} \varphi(\mathbf{x}_3) \frac{(\mathbf{x}_4 - \mathbf{x}_3)^{2n}}{(2n)!} \varphi^{(2n)}(\mathbf{x}_3) \frac{e^{i\mathbf{p}_3(\mathbf{x}_3 - \mathbf{x}_4)}}{\omega_q + \omega_3} \quad (5.35)$$

Figure 5.6: The laplacian on the φ^4 tree diagram

and using $\int d\theta (ix)^{2n} e^{i\theta x} = 2\pi \delta^{(2n)}(x)$ and $\int dx \varphi(x) \varphi^{(2n)}(x) = (-)^n \int dx \varphi^{(n)^2}(x)$ we can write an expression for the laplacian term in the Schrödinger equation correspondent to the derivatives of the quadratic term, in a local expansion:

$$\frac{(-)^{n+1} \pi}{2(2n)!} \int_{q^2 < 1/s} \int_{\mathbf{p}} \int_{\mathbf{x}} \varphi^{(n)^2}(\mathbf{x}) \frac{\delta^{(2n)}(\mathbf{p})}{\omega_{\mathbf{p}} + \omega_{\mathbf{q}}}. \quad (5.36)$$

For the six-legged diagram represented in fig.5.5, the Feynman rules give

$$\begin{aligned} & s_f g^2 \int_{\mathbf{x}_1 \dots \mathbf{x}_6 x_7 x_8} \varphi(\mathbf{x}_1) \dots \varphi(\mathbf{x}_6) \frac{\partial G_D(x_1, x_7)}{\partial t_1} \frac{\partial G_D(x_2, x_7)}{\partial t_2} \frac{\partial G_D(x_3, x_7)}{\partial t_3} \\ & \quad \times G_D(x_7, x_8) \frac{\partial G_D(x_4, x_8)}{\partial t_4} \frac{\partial G_D(x_5, x_7)}{\partial t_5} \frac{\partial G_D(x_6, x_8)}{\partial t_6} \quad (5.37) \\ & = (2i)^6 g^2 s_f \int_{\mathbf{x}_1 \dots \mathbf{x}_6 x_7 x_8} \varphi(\mathbf{x}_1) \dots \varphi(\mathbf{x}_6) \int_{p_1 \dots p_7} E_1 \dots E_6 e^{-i(p_1 + p_2 + p_3 - p_7)x_7} e^{-i(p_4 + p_5 + p_6 - p_7)x_8} \\ & \quad e^{i\mathbf{p}_1 \mathbf{x}_1} \dots e^{i\mathbf{p}_6 \mathbf{x}_6} e^{i(E_1 + E_2 + E_3 - E_7)t_7} e^{i(E_4 + E_5 + E_6)t_8} (e^{-iE_7 t_8} - e^{iE_7 t_8}) \frac{1}{\prod_{j=1}^7 p_j^2 + M^2} \quad (5.38) \end{aligned}$$

When neither end of the propagator is on the boundary $t = 0$, the image charge breaks energy conservation leading to more complicated expressions. However, for this diagram, there occurs a simplification, owing to its symmetry properties, such that we end up with delta functions in both momentum components. So, if we integrate over t_7 , we get

$$\int_{-\infty}^0 e^{i(E_1 + E_2 + E_3 - E_7)t_7} dt_7 = \frac{2\pi}{2} \delta(E_1 + E_2 + E_3 - E_7) \quad (5.39)$$

because $(E_1 + E_2 + E_3 - E_7) \rightarrow -(E_1 + E_2 + E_3 - E_7)$ is a symmetry of (5.38). On the other hand, the integral over t_8 can be simplified if we notice that

$$\int_{-\infty}^0 e^{-i(E_4 + E_5 + E_6 - E_7)t_8} dt_8 = - \int_{-\infty}^0 e^{-i(E_4 + E_5 + E_6 + E_7)t_8} dt_8 \quad (5.40)$$

in (5.38). Thus, the integrals over t_7 and t_8 give a factor proportional to

$$\frac{(2\pi)^2}{2} \delta(E_1 + E_2 + E_3 - E_7) \delta(E_4 + E_5 + E_6 + E_7) \quad (5.41)$$

Finally, integrating over $\mathbf{x}_7, \mathbf{x}_8, E_7$ and \mathbf{p}_7 , reduces (5.38) to

$$-g^2 2^5 (2\pi)^2 s_f \int_{p_1..p_6} \tilde{\varphi}(\mathbf{p}_1) \dots \tilde{\varphi}(\mathbf{p}_6) E_1 \dots E_6 \frac{\delta(\sum_{j=1}^6 \mathbf{p}_j) \delta(\sum_{k=1}^6 E_k)}{\prod_{i=1}^6 (p_i^2 + M^2) ((E_1 + E_2 + E_3)^2 + (\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3)^2 + M^2)} \quad (5.42)$$

A laborious exercise of integration over the E_i variables enable us to write a final expression for this 6-field tree diagram which just coincide with Γ_6^0 calculated earlier as it should. The symmetry factor for this diagram simplifies to $10/6!$ where the factor 10 comes from the counting of topologically distinct diagrams (i.e. labeling each leg with momentum p_i and counting the number of distinct ways this can be done) [55].

5.4 Loop Diagrams

From fig.5.7 we can work out the first order correction to the two field coefficient B_2 defined in (3.1). The diagram shown in fig.5.7(a) represents the expression

$$s_f g \int_{\mathbf{x}_1 \mathbf{x}_2 \mathbf{x}_3} \varphi(\mathbf{x}_1) \varphi(\mathbf{x}_2) \frac{\partial G_D(x_1, x_3)}{\partial t_1} G_D(x_3, x_3) \frac{\partial G_D(x_2, x_3)}{\partial t_2} \quad (5.43)$$

where

$$G_D(x_3, x_3) = \int_{p_3} \frac{(1 - e^{2it_3 E_3})}{p_3^2 + M^2} \quad (5.44)$$

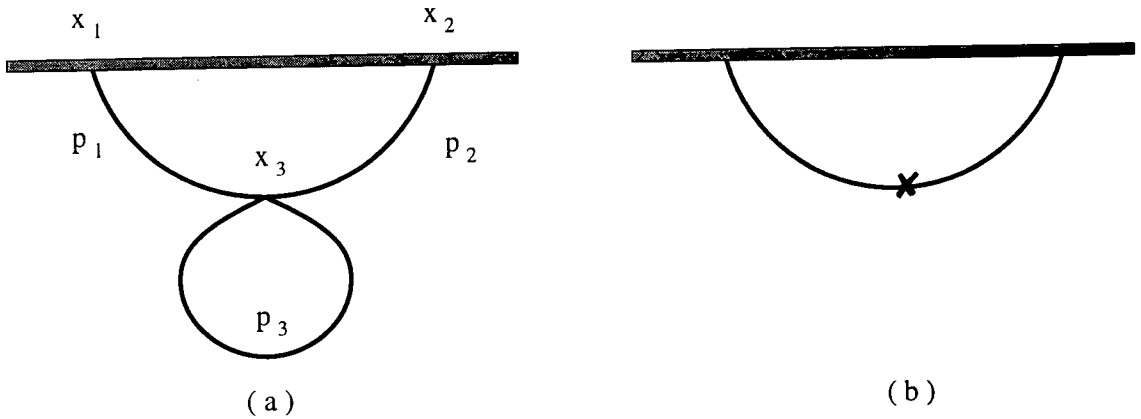


Figure 5.7:

This diagram is divergent due to the factor $G_D(x_3, x_3)$. Since this propagator does not touch the boundary, it has an energy non-conserving contribution represented by the exponential in (5.44). We regulate this integral by restricting the space-like component of the momentum such that $p_3^2 < 1/s$ just as we did for the laplacian in the Hamiltonian

(5.5). The divergence is then cancelled by a counterterm represented in fig.5.7(b) which is due to $O(\hbar)$ terms in $M^2(s)$. This process is schematically represented in fig.5.8 .

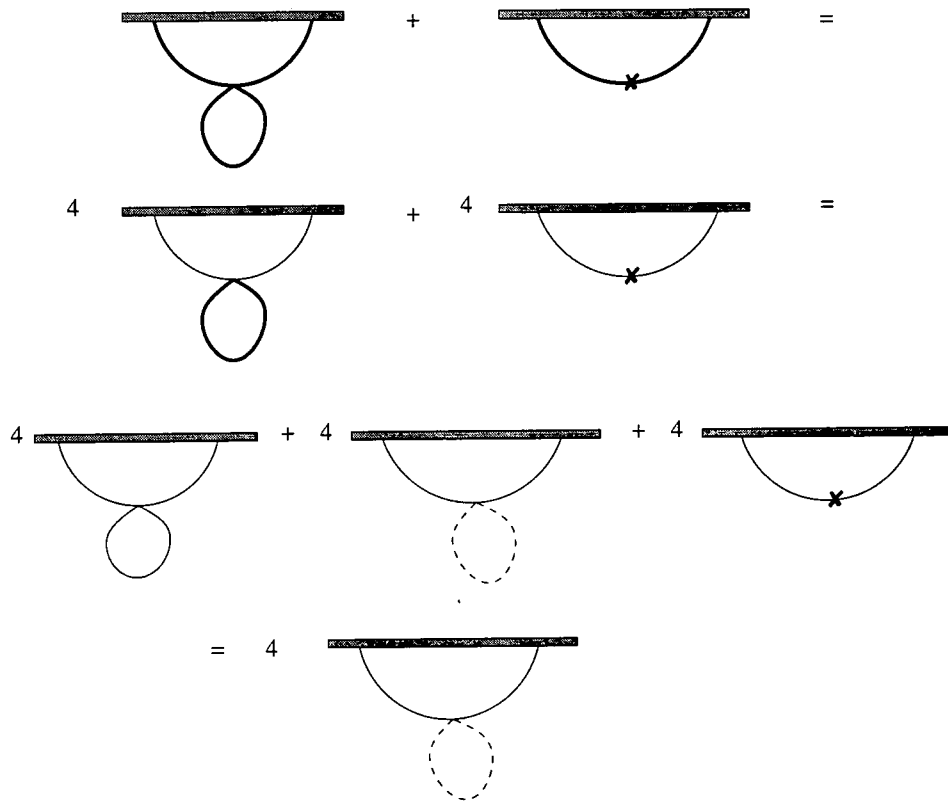


Figure 5.8:

Therefore, the finite part of equation (5.43) yields, after integrating over \mathbf{x}_3 and t_3 ,

$$8\pi^2 s_f g \int_{\mathbf{p}_1 \mathbf{p}_2 \mathbf{p}_3} \tilde{\varphi}(\mathbf{p}_1) \tilde{\varphi}(\mathbf{p}_2) E_1 E_2 \delta(\mathbf{p}_1 + \mathbf{p}_2) \delta(E_1 + E_2 - 2E_3) \frac{1}{\prod_{j=1}^3 (p_j^2 + M^2)} \quad (5.45)$$

The remaining integrations can be performed to lead to the simplified expression

$$-\frac{1}{4} s_f \int_{\mathbf{p}_1 \mathbf{p}_3} \tilde{\varphi}(\mathbf{p}_1) \tilde{\varphi}(-\mathbf{p}_1) \frac{1}{\sqrt{\mathbf{p}_3^2 + M^2} (\sqrt{\mathbf{p}_3^2 + M^2} + \sqrt{\mathbf{p}_1^2 + M^2})} \quad (5.46)$$

By setting $M = 1$ and $\mathbf{p}_1 = 0$ we can calculate B_2^{\hbar} to be $g/(16\pi)$, with $s_f = -1/4$, in agreement with equation (4.41).

The first order correction to the four-field part of W , earlier represented as Γ_4^{\hbar} , is given by the diagrams illustrated in fig.5.9(a), (b) and (c) .

The first of these diagrams translates into

$$\begin{aligned} \mathcal{A}_1 \equiv & g^2 s_f^{(a)} \int_{\mathbf{x}_1 \dots \mathbf{x}_4 \mathbf{x}_5 \mathbf{x}_6} \varphi(\mathbf{x}_1) \dots \varphi(\mathbf{x}_4) \frac{\partial G_D(x_1, x_5)}{\partial t_1} \frac{\partial G_D(x_2, x_5)}{\partial t_2} \\ & G_D(x_5, x_6) G_D(x_6, x_5) \frac{\partial G_D(x_3, x_6)}{\partial t_3} \frac{\partial G_D(x_4, x_6)}{\partial t_4} \end{aligned} \quad (5.47)$$

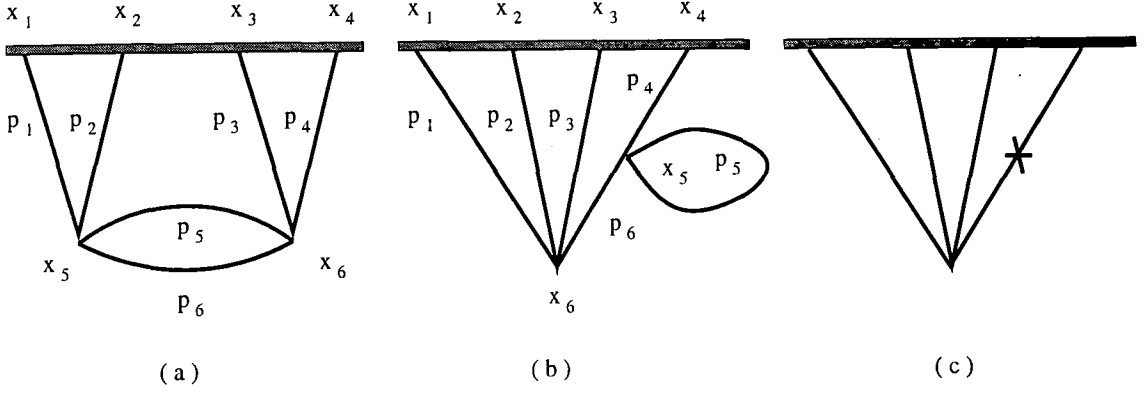


Figure 5.9: Four-field one-loop diagrams

which is written after substituting the expressions for the propagators as

$$\begin{aligned}
 & g^2 s_f^{(a)} 2^4 \int_{p_1 \dots p_6 x_5 x_6} \tilde{\varphi}(\mathbf{p}_1) \dots \tilde{\varphi}(\mathbf{p}_4) E_1 \dots E_4 e^{-ix_5(\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_6 - \mathbf{p}_5)} e^{-ix_6(\mathbf{p}_3 + \mathbf{p}_4 + \mathbf{p}_5 - \mathbf{p}_6)} \times \\
 & \times \frac{e^{-it_5(E_1 + E_2 - E_5)} (e^{-it_5 E_6} - e^{it_5 E_6}) e^{-it_6(E_3 + E_4 - E_6)} (e^{-it_6 E_5} - e^{it_6 E_5})}{\prod_{j=1}^6 p_j^2 + M^2} \quad (5.48)
 \end{aligned}$$

This expression is finite because the bubble in fig.5.9(a) does not introduce divergences in 1 + 1 dimensions. A tedious exercise of integration enable us to compute (5.48). We transcribe below the main steps of this calculation.

We start by integrating over \mathbf{x}_5 and \mathbf{x}_6 in order to get the delta function in the momenta in the space-like direction. This introduces a factor proportional to $\delta(\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_6 - \mathbf{p}_5) \delta(\mathbf{p}_3 + \mathbf{p}_4 + \mathbf{p}_5 - \mathbf{p}_6)$. Then we integrate over \mathbf{p}_6 to get $\delta(\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3 + \mathbf{p}_4)$. The integral over t_5 can also be done to reduce (5.48) to the computation of

$$\begin{aligned}
 & g^2 s_f^{(a)} 2^7 \pi^2 \int_{p_1 \dots p_5 E_6} \tilde{\varphi}(\mathbf{p}_1) \dots \tilde{\varphi}(\mathbf{p}_4) E_1 \dots E_4 \delta\left(\sum_{j=1}^4 \mathbf{p}_j\right) \delta(E_1 + E_2 + E_6 - E_5) \times \\
 & \times \frac{\int_{-\infty}^0 dt_6 e^{-it_6(E_3 + E_4)} \sin(t_6 E_5) \sin(t_6 E_6)}{\prod_{n=1}^5 (p_n^2 + M^2) (E_6^2 + (\mathbf{p}_3 + \mathbf{p}_4 + \mathbf{p}_5)^2 + M^2)} \quad (5.49)
 \end{aligned}$$

The E_3 and E_4 integrals can be readily performed to give the factor

$$\frac{e^{-|t_6|(\omega_3 + \omega_4)}}{4}$$

and the integral over t_6 ,

$$\begin{aligned}
 & \int_{-\infty}^0 dt_6 e^{t_6(\omega_3 + \omega_4)} \sin(t_6 E_5) \sin(t_6 E_6) = \\
 & \frac{(\omega_3 + \omega_4)}{2} \left(\frac{1}{(\omega_3 + \omega_4)^2 + (E_5 - E_6)^2} - \frac{1}{(\omega_3 + \omega_4)^2 + (E_5 + E_6)^2} \right) \quad (5.50)
 \end{aligned}$$

After a lengthy calculation, the integrations over E_1, E_2, E_5 and E_6 , together with the result above, simplify (5.49) to

$$\begin{aligned} \mathcal{A}_1 &= 4\pi s_f^{(a)} \int_{\mathbf{p}_1 \dots \mathbf{p}_5} \tilde{\varphi}(\mathbf{p}_1) \dots \tilde{\varphi}(\mathbf{p}_4) \delta\left(\sum_{j=1}^4 \mathbf{p}_j\right) \frac{\left(\sum_{n=1}^5 \omega_n + \bar{\omega}\right)}{\sum_{n=1}^4 \omega_n} \times \\ &\times \frac{1}{(\omega_3 + \omega_4 + \omega_5 + \bar{\omega})(\omega_1 + \omega_2 + \omega_5 + \bar{\omega})(\sum_{n=1}^4 \omega_n + 2\omega_5)(\sum_{n=1}^4 \omega_n + 2\bar{\omega})} \end{aligned} \quad (5.51)$$

where $\bar{\omega} = \sqrt{(\mathbf{p}_3 + \mathbf{p}_4 + \mathbf{p}_5)^2 + M^2}$.

Yet, there is another 4-legged- $O(\hbar)$ -diagram to be included fig.5.9(b) and the counterterm diagram associated to the renormalisation of the tadpole fig.5.9(c). Similarly to the two-field bubble diagram calculation fig.(5.7), the sum of these two diagrams amounts to the expression

$$\begin{aligned} \mathcal{A}_2 &\equiv g^2 s_f^{(b)} 2^4 \int_{p_1 \dots p_6 x_5 x_6} \tilde{\varphi}(\mathbf{p}_1) \dots \tilde{\varphi}(\mathbf{p}_4) E_1 \dots E_4 e^{-ix_6(\mathbf{p}_1 + \mathbf{p}_2 + \mathbf{p}_3 + \mathbf{p}_6)} e^{-ix_5(\mathbf{p}_4 - \mathbf{p}_6)} \\ &\times e^{-it_6(E_1 + E_2 + E_3)} (e^{-it_6 E_6} - e^{it_6 E_6}) e^{-it_5(E_4 - 2E_5 - E_6)} \frac{1}{\sum_{n=1}^6 p_n^2 + M^2} \end{aligned} \quad (5.52)$$

where we used our already familiar Feynman rules for Feynman diagrams on the Dirichlet boundary. The integrations over \mathbf{x}_5 and \mathbf{x}_6 together with an integration over \mathbf{p}_6 give the expected momentum conservation in the space-like direction, $\delta(\sum_{n=1}^4 \mathbf{p}_n)$, whereas the integrations over the time-like coordinates are similar to the previous case. Having done the integrals over E_1 to E_6 , we get to the following simplified version of (5.52):

$$\mathcal{A}_2 = -\frac{\pi}{2} g^2 s_f^{(b)} \int_{\mathbf{p}_1 \dots \mathbf{p}_5} \tilde{\varphi}(\mathbf{p}_1) \dots \tilde{\varphi}(\mathbf{p}_4) \frac{\delta\left(\sum_{n=1}^4 \mathbf{p}_n\right)}{\omega_5(\omega_4 + \omega_5)(\sum_{n=1}^4 \omega_n + 2\omega_5) \sum_{n=1}^4 \omega_n} \quad (5.53)$$

There are 3 topologically distinct diagrams associated to fig.5.9(a) [38] and 4 distinct diagrams associated to fig.5.9(b) (the bubble placed at any of the four legs). The overall symmetry factors $s_f^{(a)}$ and $s_f^{(b)}$ are respectively equal to 1/16 and 1/12. The sum $\mathcal{A}_1 + \mathcal{A}_2$ exactly reproduces the expression for Γ_4^{\hbar} we have got earlier by solving the Schrödinger equation semi-classically although the Feynman diagram method has demanded considerably more work.

Finally, the extra ϕ^6 term in the potential of the Sinh-Gordon model (see section 4.6) generates the diagram in fig.5.10.

Its analytic expression, after subtracting the counterterm represented in fig.5.10(b) reads

$$\frac{\beta^4}{96} (2\pi)^2 \int_{\mathbf{p}_1 \dots \mathbf{p}_5} \tilde{\varphi}(\mathbf{p}_1) \dots \tilde{\varphi}(\mathbf{p}_4) \frac{\delta(\sum_{n=1}^4 \mathbf{p}_n)}{\omega_5(2\omega_5 + \sum_{n=1}^4 \omega_n)} \quad (5.54)$$

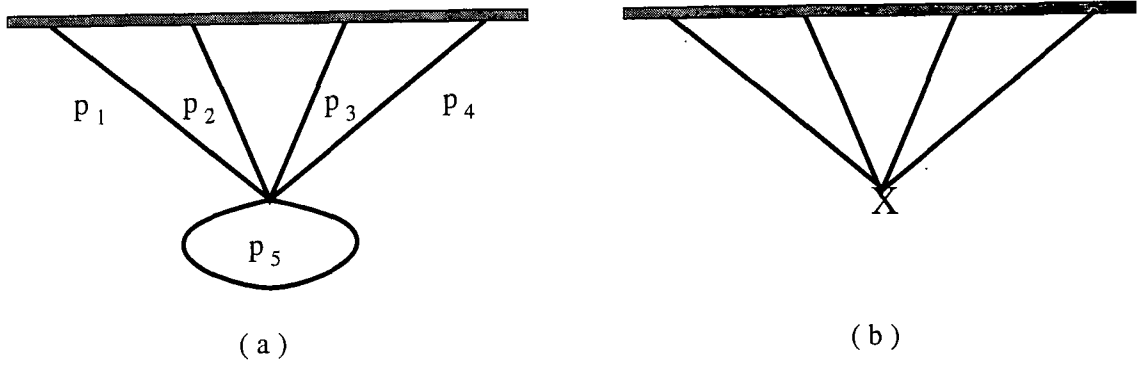


Figure 5.10: Six point interaction for the Sinh-Gordon model

for which the symmetry factor is $1/96$. This gives the modifications to the φ^4 results described in section 4.6.

Chapter 6

Applications to the Schrödinger Functional

By exploiting the analyticity properties of the Schrödinger functional, we show how a small time, local expansion in the fields can be used to construct the full functional. We also obtain the leading short-time behaviour of the Yang Mills Schrödinger functional within a local expansion in the fields.

6.1 Introduction

The Schrödinger functional for a quantum field φ in $D + 1$ space-time dimensions is the matrix element of the Euclidean time evolution operator between eigenkets of the field restricted to a D dimensional space-like surface with coordinates \mathbf{x} . It can be written as a functional integral

$$\langle \varphi | e^{-\tau H} | \bar{\varphi} \rangle = \int \mathcal{D}\tilde{\varphi} e^{-S_E[\tilde{\varphi}]} \equiv \Phi_\tau[\varphi, \bar{\varphi}] \quad (6.1)$$

where S_E is the Euclidean action for the $D + 1$ dimensional volume bounded by space-like surfaces, a time τ apart, and $\tilde{\varphi}(\mathbf{x}, 0) = \bar{\varphi}(\mathbf{x})$, $\tilde{\varphi}(\mathbf{x}, \tau) = \varphi(\mathbf{x})$ and H the corresponding Hamiltonian. Hence, the Schrödinger functional can be regarded as a euclidean quantum field theory, defined on a space time manifold with boundaries and (inhomogeneous) Dirichlet boundary conditions for the quantum fields.

Inserting a basis of eigenkets of the Hamiltonian in (6.1) shows that, at large times, it is dominated by the eigenket of lowest energy,

$$\langle \varphi | e^{-\tau H} | \varphi' \rangle \equiv \Psi[\varphi] \Psi^*[\varphi'] e^{-\tau E_0} \quad , \quad (6.2)$$

where $\Psi[\varphi] = \langle \varphi|0 \rangle$ is the vacuum functional.

As we have described in the previous chapters, the logarithm of the vacuum functional ($\ln \Psi[\varphi] = W[\varphi]$) is, in perturbation theory, a sum of connected Feynman diagrams and in general a non-local functional. If φ varies slowly on a length scale of the inverse of the lightest mass in the theory, $W[\varphi]$ reduces to a sum of local functionals. Therefore, the study of the scaling and analyticity properties of W has enabled us to reconstruct it from its local expansion whose coefficients are determined by a suitably constructed Schrödinger equation. In other words, we have translated the eigenvalue problem of the Hamiltonian into an infinite set of algebraic equations for the coefficients of the local expansion. By truncating the expansion, we have a new approximation scheme which offers the possibility of solution beyond perturbation theory in the couplings [2]. This scheme is especially adequate for theories in which mass is generated quantum mechanically.

For theories that are classically massive, the local expansion appears already within the framework of standard semi-classical perturbation theory but for Yang-Mills theory for example, which is classically massless, the leading order contribution to W does not reduce to a local expansion for slowly varying fields. Nonetheless quantum effects generate a non-zero mass-gap and so the full expression for W does have such an expansion, as has been seen in Monte-Carlo simulations of lattice gauge theory [43],[44],[41]. In principle this will be determined by solving the Schrödinger equation, but in practice the construction of this equation to a sufficient order to generate reliable results is some way off: it involves the construction of a Laplacian that respects gauge invariance and is amenable for computations. It would have been useful to study this local expansion using standard semi-classical techniques. As we cannot, we will study instead the the Schrödinger functional

$$\begin{aligned} \Phi_\tau[\mathbf{A}, \mathbf{A}'] &= \langle \mathbf{A} | e^{-H\tau/\hbar} | \mathbf{A}' \rangle, \\ H[\mathbf{A}, \mathbf{E}] &= -\frac{1}{2g^2} \int d^3\mathbf{x} \operatorname{tr}(\mathbf{B}^2 + \mathbf{E}^2) \end{aligned} \quad (6.3)$$

where $\mathbf{E} = -\dot{\mathbf{A}}$, $\mathbf{B} = \nabla \wedge \mathbf{A} + \mathbf{A} \wedge \mathbf{A}$, $\mathbf{A} = \mathbf{A}^A T^A$, $\operatorname{tr}(T^A T^B) = -\delta^{AB}$, $[T^A, T^B] = f^{ABC} T^C$ and we work in the Weyl gauge, $A_0 = 0$.

Again, the logarithm of this functional, $W_\tau[\mathbf{A}, \mathbf{A}']$ is a sum of connected diagrams, and is non-local, but having introduced the length-scale τ (which acts as an infra-red cut-off) into the problem results in a local expansion for fields that vary slowly, even within the



semi-classical expansion. In other words we can compute the Schrödinger functional for the short-time behaviour using both a local expansion, and semi-classical perturbation theory. This enables us to compare the efficacy of solving the problem in two different ways, i.e. by solving the Hamilton-Jacobi equation for the derivative expansion and by evaluating the leading order contribution to the functional integral. The result of the semi-classical calculation is useful as it will still be a good leading order approximation to the full expression for times that are small in comparison to the inverse of the lightest glueball mass. Furthermore we can show that by studying its analyticity properties, one can reconstruct the Schrödinger functional from its small time expansion [65],[3],[4].

6.2 Reconstructing the Schrödinger Functional

Consider the free scalar theory in 1 + 1 dimensions. The Hamiltonian is written

$$H = \int dx \frac{1}{2} (\pi^2 + \varphi'^2 + m^2 \varphi^2). \quad (6.4)$$

We can adopt the following ansatz for the Schrödinger functional,

$$\Phi_\tau[\varphi, \bar{\varphi}] = \prod_p D(p, \tau) e^{W_\tau[\varphi, \bar{\varphi}]} \quad (6.5)$$

where W can be written as

$$\begin{aligned} W_\tau[\varphi, \bar{\varphi}] &= \int dp \varphi(p) \varphi(-p) \Gamma_1(p, \tau) + \int dp \varphi(p) \bar{\varphi}(-p) \Gamma_2(p, \tau) \\ &+ \int dp \bar{\varphi}(p) \bar{\varphi}(-p) \Gamma_3(p, \tau) \end{aligned} \quad (6.6)$$

since the Hamiltonian is quadratic. $\varphi(p)$ is the Fourier transform of $\varphi(x)$ and $D(p, \tau)$ is proportional to $(\det(-\partial_x^2 + \omega^2))^{-\frac{1}{2}}$ where $\omega = p^2 + m^2$. This is in complete analogy with the harmonic oscillator path integral [38]. We can fully determine Φ since it satisfies the Schrödinger equation in the momentum space.

$$\begin{aligned} \int dk 2\pi \left(\frac{\delta^2 W}{\delta\varphi(-k) \delta\varphi(k)} + \frac{\delta W}{\delta\varphi(k)} \frac{\delta W}{\delta\varphi(-k)} \right) - \int \frac{dk}{2\pi} (k^2 + m^2) \varphi(k) \varphi(-k) \\ - 2 \frac{\dot{D}}{D} - 2 \dot{W} = 0 \end{aligned} \quad (6.7)$$

(where the dot stands for differentiation with respect to τ) with initial condition

$$\lim_{\tau \rightarrow 0} \Phi_\tau[\varphi, \bar{\varphi}] = \delta[\varphi - \bar{\varphi}]. \quad (6.8)$$

Moreover since $W_\tau[\varphi, \bar{\varphi}] = W_\tau[\bar{\varphi}, \varphi]$ we have $\Gamma_1 = \Gamma_3$. Taking (6.6) into the Schrödinger equation yields a set of coupled differential equations, namely

$$\begin{aligned} 8\pi\Gamma_1^2 - \frac{(k^2 + m^2)}{2\pi} - 2\dot{\Gamma}_1 &= 0, \\ 8\pi\Gamma_1\Gamma_2 - 2\dot{\Gamma}_2 &= 0, \\ 2\pi\Gamma_2^2 - 2\dot{\Gamma}_1 &= 0 \text{ and} \\ 2\pi\Gamma_1 - \frac{\dot{D}}{D} &= 0. \end{aligned} \quad (6.9)$$

The first of these equations is a non-linear Riccati type differential equation ($\dot{y} - a^2y^2 + b^2 = 0$), which in turn can be linearised by the change of variables $y = b/a + 1/z$ and easily solved to give the well known results

$$\begin{aligned} \Gamma_1 &= \frac{\omega (e^{-2\omega\tau} + 1)}{4\pi (e^{-2\omega\tau} - 1)}, \\ \Gamma_2 &= \frac{\omega \cdot 4e^{-\omega\tau}}{4\pi (e^{-2\omega\tau} - 1)}, \\ D &= \sqrt{\frac{\omega}{\pi(e^{\omega\tau} - e^{-\omega\tau})}}. \end{aligned} \quad (6.10)$$

As a final check, note that in the limit $\tau \rightarrow \infty$, Γ_2 vanishes whereas Γ_1 and D allow us to rewrite the Schrödinger functional as

$$\prod_p \left(\frac{\omega}{\pi}\right)^{1/2} e^{-\omega/2} \exp\left(\int \frac{dp}{2\pi} \frac{\omega}{2} (\varphi^2(p) + \bar{\varphi}^2(p))\right) \quad (6.11)$$

from which, if we recall (6.2), we can read off the vacuum functional

$$\Psi_0[\varphi] = \prod_p \left(\frac{\omega}{\pi}\right)^{1/4} \exp\left(-\frac{1}{2} \frac{\omega}{2\pi} \varphi(p)\varphi(-p)\right) \quad (6.12)$$

and the vacuum energy density $\mathcal{E}_0 = \int dp \omega/2$.

Notice that a small τ expansion of Γ_1 , for example, leads to a local derivative expansion in the fields which makes sense when the field varies slowly on the scale of τ , even when $m = 0$, namely $\int dp \varphi \Gamma_1 \varphi = \int dx \left(-\frac{1}{\tau} \varphi^2(x) - \frac{\tau}{3} \varphi'^2 + \frac{\tau^3}{45} \varphi''^2 + \dots\right)$. As a matter of illustration let us suppose that we want to construct the Schrödinger functional out of a small time, local expansion in the fields. Taking (6.8) into account, we can start out with

$$\begin{aligned} W &= \int dk \left(\frac{b_0}{\tau} (\varphi(k)\varphi(-k) - 2\varphi(k)\bar{\varphi}(-k) + \bar{\varphi}(k)\bar{\varphi}(-k)) + (b_1\tau k^2 + b_2\tau^3 k^4 + \dots) \times \right. \\ &\times \left. (\varphi(k)\varphi(-k) + \bar{\varphi}(k)\bar{\varphi}(-k)) + (c_0\tau k^2 + c_1\tau^3 k^4 + \dots) \varphi(k)\bar{\varphi}(-k) \right) \end{aligned} \quad (6.13)$$

and expansion coefficients b_0, b_1 , etc. are determined by the Schrödinger equation. For instance, the terms which depend only on φ can be solved to give

$$\int dk \frac{1}{4\pi} \varphi(k) \left(-\frac{1}{\tau} - \frac{1}{3}k^2\tau + \frac{1}{45}k^4\tau^3 - \dots \right) \varphi(-k). \quad (6.14)$$

If (6.1) is evaluated for a scaled Euclidean time $\tau = t/\sqrt{s}$, it extends to an analytic function of s with cuts restricted to the negative real axis. Therefore, we can use Cauchy's theorem to related the large- s , or equivalently, small- τ behaviour to the $s = 1$ value:

$$\Phi_\tau = \lim_{\lambda \rightarrow \infty} \frac{1}{2\pi i} \int_{|s|=\infty} \frac{ds}{s-1} e^{\lambda(s-1)} \Phi_{\frac{t}{\sqrt{s}}}. \quad (6.15)$$

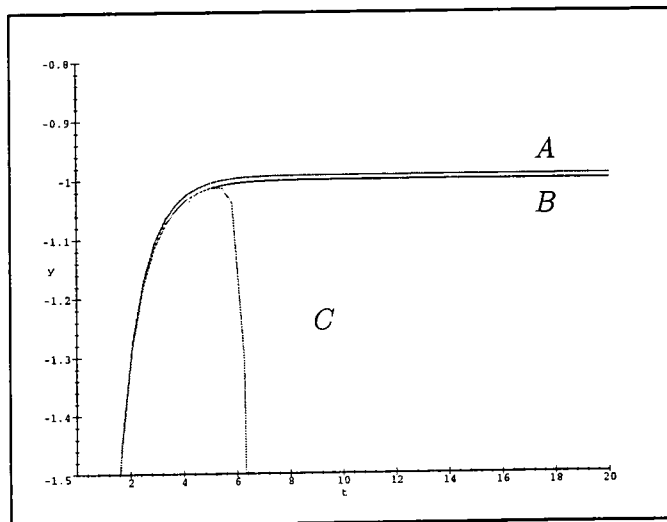
The exponential term removes the contribution from the cut as $\lambda \rightarrow \infty$ and the small- τ expansion of Φ_τ can be used in the right hand side of (6.15). An approximation scheme in which one works with a finite number of terms and a large but finite value of λ in this series has been shown to be successful [4]. Following these steps (6.14) can be evaluated to give

$$4\pi S(\lambda, t) = \frac{1}{\sqrt{\pi}} \left(\frac{-1}{t\sqrt{\lambda}} - \left(\frac{1}{t} + \frac{1}{6}t\right)\sqrt{\lambda} + \frac{4}{3}\left(\frac{1}{4}t + \frac{1}{12}t + \frac{1}{360}t^3\right)\lambda^{3/2} + \dots + \frac{(-2)^{(n+1)/2}}{n(n-2)(n-4)\dots 1} \times \right. \\ \left. \left(\frac{(n-2)(n-4)\dots 1}{(n+1)(n-1)\dots 4} \frac{1}{t} + \frac{(n-2)(n-4)\dots 1}{(n-1)(n-3)\dots 2} \frac{1}{6}t + \frac{(n-2)(n-4)\dots 3}{(n-3)(n-5)\dots 2} \frac{1}{360}t^3 + \dots + O(t^n) \right) \lambda^{n/2} + \dots \right) \quad (6.16)$$

where we have set $k = 1$. The graph in fig:(6.1) illustrates the resummation of the small τ expansion.

The curve A is (6.16) truncated to 14 terms. The value of λ is chosen so that the last term included is one per cent of the value of the series. This curve should be compared with the curve B which is the plot of $4\pi\Gamma_1$, the function to which the series should converge, and finally curve C is a plot of (6.14) also truncated to 14 terms so as to show that by means of the re-summed series for small τ we can reconstruct the Schrödinger functional for any τ .

For abelian gauge field theory we would have obtained similar results. The basic difference is that we should also impose gauge invariance under spatial gauge transformations so as to satisfy the Gauss's law constraint. This constraint introduces some complications in defining the path integral representation of the Schrödinger functional, more specifically in the definition of the measure. Roughly speaking, we have an infinity coming from integrating gauge equivalent components of the gauge potential. For the abelian gauge

Figure 6.1: Resummation of the small τ expansion

fields, this infinite is easily factored out and absorbed into the normalisation whereas for the non-abelian case this is healed by the well known Faddeev-Popov prescription. As we are mainly interested in the gauge potential dependence of the Schrödinger functional, we will not worry about this subtlety in our present analysis.

Thus we can write

$$\begin{aligned}
 W &= \int \frac{d^3 \mathbf{p}}{(2\pi)^3} \mathbf{A}_T(\mathbf{p}) \mathbf{A}_T(-\mathbf{p}) \Gamma_1(|\mathbf{p}|, \tau) + \mathbf{A}_T(\mathbf{p}) \bar{\mathbf{A}}_T(-\mathbf{p}) \Gamma_2(|\mathbf{p}|, \tau) \\
 &+ \bar{\mathbf{A}}_T(\mathbf{p}) \bar{\mathbf{A}}_T(-\mathbf{p}) \Gamma_1(|\mathbf{p}|, \tau) .
 \end{aligned} \tag{6.17}$$

where A_T is the transversal, physical component of the gauge potential, namely

$$\mathbf{A}_T(\mathbf{p}) = \mathbf{A}(\mathbf{p}) - \frac{(\mathbf{p} \cdot \mathbf{A}(\mathbf{p})) \mathbf{p}}{|\mathbf{p}|^2} \tag{6.18}$$

Substituting (6.17) into the Schrödinger equation $H e^W + \partial e^W / \partial \tau = 0$ where H is the abelian version of (6.3), we get the same expressions for Γ_1 and Γ_2 as we obtained for the free scalar field. As before, the large τ limit gives us the free photon vacuum functional

$$\Psi_0[\mathbf{A}] \sim \exp\left\{-\frac{1}{2} \int \frac{d^3 p}{(2\pi)^3} \frac{(\mathbf{p} \wedge \mathbf{A}(\mathbf{p})) \cdot (\mathbf{p} \wedge \mathbf{A}(-\mathbf{p}))}{|\mathbf{p}|}\right\} \tag{6.19}$$

which, in the coordinate space, becomes

$$\Psi_0[\mathbf{A}] \sim \exp\left\{-\frac{1}{2} \int d^3 \mathbf{x} \int d^3 \mathbf{y} \mathbf{B}(\mathbf{x}) \cdot \mathbf{B}(\mathbf{y}) \Delta(\mathbf{x} - \mathbf{y})\right\} \tag{6.20}$$

with $\Delta(\mathbf{x} - \mathbf{y}) = 1/(2\pi^2(\mathbf{x} - \mathbf{y})^2)$.

6.3 Leading Order Yang-Mills Schrödinger Functional

We follow the same scheme for the differential equation approach to $W_\tau[\mathbf{A}, \mathbf{A}']$. Φ_τ satisfies the Schrödinger equation with initial condition

$$-\hbar \frac{\partial}{\partial \tau} \Phi_\tau[\mathbf{A}, \mathbf{A}'] = H \Phi_\tau[\mathbf{A}, \mathbf{A}'], \quad \lim_{\tau \rightarrow 0} \Phi_\tau[\mathbf{A}, \mathbf{A}'] = \delta[\mathbf{A} - \mathbf{A}'] \quad (6.21)$$

In the Schrödinger representation the Yang-Mills electric field is represented by

$$\hat{E}_C^\mu(\mathbf{x}) = i\hbar g^2 \frac{\delta}{\delta A_\mu^C(\mathbf{x})}, \quad (6.22)$$

so that

$$H = \left(-\frac{1}{2} \hbar g^2 \Delta + g^{-2} \mathcal{B} \right), \quad \Delta \equiv \int d^3\mathbf{x} \frac{\delta}{\delta \mathbf{A}^C(\mathbf{x})} \cdot \frac{\delta}{\delta \mathbf{A}^C(\mathbf{x})}$$

and

$$\mathcal{B} = -\frac{1}{2} \int d^3\mathbf{x} \operatorname{tr} \mathbf{B}^2. \quad (6.23)$$

The Schrödinger equation must be regularized as the kinetic term Δ contains two functional derivatives acting at the same point of space, however this will not affect the leading order calculation, since if we set $W_\tau[\mathbf{A}, \mathbf{A}'] = w[\mathbf{A}, \mathbf{A}'] / (\hbar g^2)$ the Schrödinger equation reads:

$$\frac{1}{2} \hbar g^2 \Delta w + \frac{g^2}{2} \left(\int d^3\mathbf{x} \frac{\delta w}{\delta \mathbf{A}^C} \cdot \frac{\delta w}{\delta \mathbf{A}^C} \right) + \mathcal{B} + \frac{\partial w}{\partial \tau} = 0. \quad (6.24)$$

Neglecting the $O(\hbar g^2)$ term leads to the Hamilton-Jacobi equation which we now solve in a derivative expansion subject to the conditions that $w[\mathbf{A}, \mathbf{A}']$ be real and invariant under simultaneous time-independent gauge transformations of \mathbf{A} and \mathbf{A}' and that $w[\mathbf{A}, \mathbf{A}'] = w[\mathbf{A}', \mathbf{A}]$.

If we order the local expansion of w according to the mass dimension of local functionals, then the first gauge invariant term is

$$\int d^3\mathbf{x} \operatorname{tr} \mathcal{A}^2 a(\tau), \quad (6.25)$$

where $\mathcal{A} \equiv \mathbf{A} - \mathbf{A}'$. Since the only length-scale in this classical problem is τ this enters w multiplied by $1/\tau$, leaving possibly a constant to be determined. This term will enable us to fit the initial condition since as τ becomes small $\exp \tau^{-1} \int d^3\mathbf{x} \operatorname{tr} \mathcal{A}^2 \sim \delta[\mathbf{A} - \mathbf{A}']$. Next we must include dimension four fields, for example

$$\int d^3\mathbf{x} \operatorname{tr} \mathbf{B}^2 b(\tau) \quad (6.26)$$

which is needed to cancel a similar term in the Hamiltonian. Notice that such term does not contain \mathbf{A}' and hence violates the symmetry of interchanging \mathbf{A}' and \mathbf{A} . We will soon impose this symmetry within our ansatz and thereof obtain relations between the coefficients of its terms. The Hamilton-Jacobi equation generates cross-terms from these two functionals of the form

$$\left(\frac{\delta}{\delta A_\mu^R(\mathbf{x})} \int d^3 \mathbf{x}' \mathcal{A}_\nu^A(\mathbf{x}') \mathcal{A}_\nu^A(\mathbf{x}') \right) \left(\frac{\delta}{\delta A_\mu^R(\mathbf{x})} \frac{1}{2} \int d^3 \mathbf{x}' B_\rho^A(\mathbf{x}') B_\rho^A(\mathbf{x}') \right) \quad (6.27)$$

$$= \left(2 \mathcal{A}_\mu^R|_x \right) \left(\mathcal{D}_{\mu\rho}^{RA} B_\rho^A|_x \right) \quad (6.28)$$

where

$$\mathcal{D}_{\mu\rho}^{RA} \equiv \epsilon_{\mu\alpha\rho} D_\alpha^{RA} \quad , \quad D_\alpha^{RA} = (\partial_\alpha \delta^{AR} + f^{RSA} A_\alpha^S) . \quad (6.29)$$

which results, in a shortened notation

$$\int d^3 \mathbf{x} \operatorname{tr} \mathcal{A} \cdot \mathcal{D} \mathbf{B} |_x . \quad (6.30)$$

This is a gauge-invariant dimension four term that should be included in the expansion of w (as too should all further terms generated by repeated applications of $\int d^3 \mathbf{x} \mathcal{A} \cdot \delta / \delta \mathbf{A}$).

By making use of the following relations

$$\begin{aligned} & \int d^3 \mathbf{x} \mathcal{A}^C(\mathbf{x}) \cdot \frac{\delta}{\delta \mathbf{A}^C(\mathbf{x})} \int d^3 \mathbf{x}' \mathcal{A}_\mu^A \mathcal{D}_{\mu\rho}^{AR} B_\rho^R|_{x'} = \\ & \int d^3 \mathbf{x} \mathcal{A}_\mu^A \mathcal{D}_{\mu\rho}^{AR} B_\rho^R|_x + \int \int d^3 \mathbf{x} d^3 \mathbf{y} \mathcal{A}_\mu^A(\mathbf{x}) \Lambda_{\mu\nu}^{AB}(\mathbf{x}, \mathbf{y}) \mathcal{A}_\nu^B(\mathbf{y}) , \end{aligned} \quad (6.31)$$

where

$$\begin{aligned} \Lambda_{\mu\nu}^{AB}(\mathbf{x}, \mathbf{y}) &= \frac{\delta}{\delta A_\mu^A(\mathbf{x})} \frac{\delta}{\delta A_\nu^B(\mathbf{y})} \frac{1}{2} \int d^3 \mathbf{x}' B_\rho^R B_\rho^R|_{x'} \\ &= (\mathcal{D}_{\mu\rho}^{AR} \mathcal{D}_{\rho\nu}^{RB} | + f^{ABR} \epsilon_{\mu\nu\rho} B_\rho^R)|_x \delta^3(\mathbf{x} - \mathbf{y}) \\ &= (\mathcal{D}_{\mu\rho}^{AR} \mathcal{D}_{\rho\nu}^{RB} + F_{\mu\nu}^{AB})|_x \delta^3(\mathbf{x} - \mathbf{y}) ; \end{aligned} \quad (6.32)$$

$$\begin{aligned} & \int d^3 \mathbf{x}' \mathcal{A}^C(\mathbf{x}') \cdot \frac{\delta}{\delta \mathbf{A}^C(\mathbf{x}')} \int \int d^3 \mathbf{x} d^3 \mathbf{y} \mathcal{A}_\mu^A(\mathbf{x}) \Lambda_{\mu\nu}^{AB}(\mathbf{x}, \mathbf{y}) \mathcal{A}_\nu^B(\mathbf{y}) = \\ & 2 \int \int d^3 \mathbf{x} d^3 \mathbf{y} \mathcal{A}_\mu^A(\mathbf{x}) \Lambda_{\mu\nu}^{AB}(\mathbf{x}, \mathbf{y}) \mathcal{A}_\nu^B(\mathbf{y}) + 6 \int d^3 \mathbf{x} (D_\mu \mathcal{A}_\nu)^A ([\mathcal{A}_\mu, \mathcal{A}_\nu])^A|_x ; \end{aligned} \quad (6.33)$$

$$\begin{aligned} & \int d^3 \mathbf{x}' \mathcal{A}^C(\mathbf{x}') \cdot \frac{\delta}{\delta \mathbf{A}^C(\mathbf{x}')} \int d^3 \mathbf{x} (D_\mu \mathcal{A}_\nu)^A [\mathcal{A}_\mu, \mathcal{A}_\nu]^A|_x = \\ & 3 \int d^3 \mathbf{x} (D_\mu \mathcal{A}_\nu)^A [\mathcal{A}_\mu, \mathcal{A}_\nu]^A|_x + \int d^3 \mathbf{x} [\mathcal{A}_\mu, \mathcal{A}_\nu]^A [\mathcal{A}_\mu, \mathcal{A}_\nu]^A|_x \end{aligned} \quad (6.34)$$

we exhaust the terms up to dimension four whilst our ansatz is enlarged to

$$\begin{aligned}
W_\tau[\mathbf{A}, \mathbf{A}'] &= \int d^3\mathbf{x} \operatorname{tr} \{ \mathcal{A}^2 a/\tau + \mathbf{B}^2 b \tau + \mathcal{A} \cdot \mathcal{D}B c \tau \\
&+ \int d^3\mathbf{y} \mathcal{A}(\mathbf{x}) \cdot \Lambda(\mathbf{x}, \mathbf{y}) \cdot \mathcal{A}(\mathbf{y}) d \tau + D\mathcal{A} \cdot [\mathcal{A}, \mathcal{A}] e \tau \\
&+ [\mathcal{A}, \mathcal{A}] \cdot [\mathcal{A}, \mathcal{A}] f \tau \}
\end{aligned} \tag{6.35}$$

in which the τ dependence was inferred by dimensional analysis, leaving arbitrary constants to be determined. We start out by imposing $w[\mathbf{A}, \mathbf{A}'] = w[\mathbf{A}', \mathbf{A}]$. Since $w[\mathbf{A}, \mathbf{A}'] = w[\mathbf{A}, \mathcal{A}]$, this condition can be equally expressed as

$$W[\mathbf{A}, \mathcal{A}] = W[\mathbf{A}', -\mathcal{A}]. \tag{6.36}$$

To build the right hand side of (6.36), we expand each term of (6.35) in the primed variables which results :

$$\begin{aligned}
\int d^3\mathbf{x} \operatorname{tr} \mathbf{B}^2|_x &= \int d^3\mathbf{x} \operatorname{tr} \{ \mathbf{B}'^2|_x + 2 \mathcal{A} \cdot \mathcal{D}'B'|_x + \int d^3\mathbf{y} \mathcal{A}(\mathbf{x}) \cdot \Lambda'(\mathbf{x}, \mathbf{y}) \cdot \mathcal{A}(\mathbf{y}) \\
&+ 2D'_\mu \mathcal{A}_\nu [\mathcal{A}_\mu, \mathcal{A}_\nu]|_x + \frac{1}{2} [\mathcal{A}_\mu, \mathcal{A}_\nu] [\mathcal{A}_\mu, \mathcal{A}_\nu]|_x \},
\end{aligned} \tag{6.37}$$

$$\begin{aligned}
\int d^3\mathbf{x} \operatorname{tr} \mathcal{A} \cdot \mathcal{D}B &= \int d^3\mathbf{x} \operatorname{tr} \{ \mathcal{A} \cdot \mathcal{D}'B'|_x + \int d^3\mathbf{y} \mathcal{A}(\mathbf{x}) \cdot \Lambda'(\mathbf{x}, \mathbf{y}) \cdot \mathcal{A}(\mathbf{y}) \\
&+ 3 D'_\mu \mathcal{A}_\nu [\mathcal{A}_\mu, \mathcal{A}_\nu]|_x + [\mathcal{A}_\mu, \mathcal{A}_\nu] [\mathcal{A}_\mu, \mathcal{A}_\nu]|_x \},
\end{aligned} \tag{6.38}$$

$$\begin{aligned}
\int \int d^3\mathbf{x} d^3\mathbf{y} \operatorname{tr} \mathcal{A}(\mathbf{x}) \cdot \Lambda(\mathbf{x}, \mathbf{y}) \cdot \mathcal{A}(\mathbf{y}) &= \int \int d^3\mathbf{x} d^3\mathbf{y} \operatorname{tr} \mathcal{A}(\mathbf{x}) \cdot \Lambda'(\mathbf{x}, \mathbf{y}) \cdot \mathcal{A}(\mathbf{y}) \\
&+ \int d^3\mathbf{x} \operatorname{tr} \{ 6D'_\mu \mathcal{A}_\nu [\mathcal{A}_\mu, \mathcal{A}_\nu]|_x \\
&+ 3[\mathcal{A}_\mu, \mathcal{A}_\nu] [\mathcal{A}_\mu, \mathcal{A}_\nu]|_x \},
\end{aligned} \tag{6.39}$$

$$\int d^3\mathbf{x} \operatorname{tr} D_\mu \mathcal{A}_\nu [\mathcal{A}_\mu, \mathcal{A}_\nu]|_x = \int d^3\mathbf{x} \operatorname{tr} D'_\mu \mathcal{A}_\nu [\mathcal{A}_\mu, \mathcal{A}_\nu]|_x + [\mathcal{A}_\mu, \mathcal{A}_\nu] [\mathcal{A}_\mu, \mathcal{A}_\nu]|_x. \tag{6.40}$$

Therefore, in order to preserve (6.36), we must have

$$\begin{aligned}
c &= -b \\
e &= \frac{1}{2}b - 3d.
\end{aligned} \tag{6.41}$$

Finally, if we substitute (6.35) into the Hamilton-Jacobi equation the remaining coefficients are determined leading to our final result for W :

$$\begin{aligned}
W_\tau[\mathbf{A}, \mathbf{A}'] &= \frac{1}{2\hbar g^2} \int d^3\mathbf{x} \operatorname{tr} \left\{ -\frac{\mathcal{A}^2}{\tau} - \mathbf{B}^2 \tau + \mathcal{A} \cdot \mathcal{D}B \tau \right. \\
&- \int d^3\mathbf{y} \mathcal{A}(\mathbf{x}) \cdot \Lambda(\mathbf{x}, \mathbf{y}) \cdot \mathcal{A}(\mathbf{y}) \frac{\tau}{3} + D\mathcal{A} \cdot [\mathcal{A}, \mathcal{A}] \frac{\tau}{2} \\
&- [\mathcal{A}, \mathcal{A}] \cdot [\mathcal{A}, \mathcal{A}] \frac{\tau}{10} \left. \right\}.
\end{aligned} \tag{6.42}$$

We will now compute this expression using a different method, so as to gauge the efficiency of the above approach. The functional integral representation of $W_\tau[\mathbf{A}_{out}, \mathbf{A}_{in}]$ leads to a saddle-point approximation in which this is given to leading order by minus the Euclidean action

$$\frac{1}{2g^2} \int d^3\mathbf{x} dt (\mathbf{E}^A(\mathbf{x}) \cdot \mathbf{E}^A(\mathbf{x}) + \mathbf{B}^A(\mathbf{x}) \cdot \mathbf{B}^A(\mathbf{x})) \quad (6.43)$$

where, in the temporal gauge,

$$\mathbf{E} = -\dot{\mathbf{A}} \quad , \quad \mathbf{B} = \nabla \wedge \mathbf{A} + \mathbf{A} \wedge \mathbf{A} \quad . \quad (6.44)$$

The fields \mathbf{A} are required to be on-shell, i.e. they satisfy the Euler Lagrange equations

$$\ddot{\mathbf{A}} = -D \wedge \mathbf{B} \quad , \quad D \wedge \mathbf{B} = \nabla \wedge \mathbf{B} + \mathbf{A} \wedge \mathbf{B} + \mathbf{B} \wedge \mathbf{A} \quad (6.45)$$

subject to the boundary conditions that at $\mathbf{A}(\mathbf{x}, 0) = \mathbf{A}_{in}$ and $\mathbf{A}(\mathbf{x}, \tau) = \mathbf{A}_{out}$. We want to calculate S_E as an expansion in dimension of the fields but since the coupling constant is dimensionless in $(3+1)$ -dimensional space-time, this is the same as an expansion in increasing powers of τ . If we expand the gauge potential as a power series in t

$$\mathbf{A}(\mathbf{x}, t) = \sum_{n=0}^{\infty} \mathbf{A}_n(\mathbf{x}) t^n \quad , \quad (6.46)$$

the Euler Lagrange equations turn into

$$\sum_{n=0}^{\infty} (n+1)(n+2) \mathbf{A}_{n+2}(\mathbf{x}) t^n = -D \wedge \mathbf{B} \quad . \quad (6.47)$$

Thus $\mathbf{A}_{in} = \mathbf{A}_0$ and by calling \mathbf{A}_{out} simply \mathbf{A} and $\mathcal{A} = \mathbf{A} - \mathbf{A}_0$, we can express \mathbf{A}_1 as

$$\mathbf{A}_1 = \frac{\mathcal{A}}{\tau} - \tau \mathbf{A}_2 - \tau^2 \mathbf{A}_3 - \dots \quad . \quad (6.48)$$

So A_0 and A_1 are determined by the boundary conditions while the others A_n will be determined in terms of them using (6.47). To calculate the other terms, we equate powers of t on both sides of (6.47) to obtain

$$\begin{aligned} \mathbf{A}_0 &= \mathbf{A}_{in} \\ \mathbf{A}_1 &= \frac{\mathcal{A}}{\tau} - \mathbf{A}_2 \tau - \mathbf{A}_3 \tau^2 - \mathbf{A}_4 \tau^3 - \mathbf{A}_5 \tau^4 - O(\tau^2) \quad , \\ \mathbf{A}_2 &= -\frac{1}{2} D_0 \wedge \mathbf{B}_0 \quad , \\ \mathbf{A}_3 &= -\frac{1}{6\tau} \{ D_0 \wedge (D_0 \wedge \mathcal{A}) + \mathcal{A} \wedge \mathbf{B}_0 + \mathbf{B}_0 \wedge \mathcal{A} \} \quad , \\ \mathbf{A}_4 &= -\frac{1}{12\tau^2} \{ D_0 \wedge (\mathcal{A} \wedge \mathcal{A}) + \mathcal{A} \wedge (D_0 \wedge \mathcal{A}) + (D_0 \wedge \mathcal{A}) \wedge \mathcal{A} \} \quad , \\ \mathbf{A}_5 &= -\frac{1}{20\tau^3} \{ \mathcal{A} \wedge (\mathcal{A} \wedge \mathcal{A}) + (\mathcal{A} \wedge \mathcal{A}) \wedge \mathcal{A} \} \quad . \end{aligned} \quad (6.49)$$

where we neglected terms of $O(L^{-n})$ $n > 4$ and $D_0 \wedge = \nabla \wedge + \mathbf{A}_0 \wedge + \wedge \mathbf{A}_0$. The subscript 0 denotes that the gauge potential has been taken as \mathbf{A}_0 , and $\mathcal{A} = \mathbf{A}_{out} - \mathbf{A}_{in}$. Thus the magnetic and electric terms in the Yang Mills action can be rewritten, after some considerable algebra, as

$$\begin{aligned} \mathbf{B} \cdot \mathbf{B} &= \mathbf{B}_0 \cdot \mathbf{B}_0 + \frac{t}{T} \{2 (D_0 \wedge \mathcal{A}) \cdot \mathbf{B}_0\} \\ &+ \frac{t^2}{T^2} \{(D_0 \wedge \mathcal{A}) \cdot (D_0 \wedge \mathcal{A}) + 2\mathbf{B}_0 \cdot (\mathcal{A} \wedge \mathcal{A})\} + \frac{t^3}{T^3} \{2(D_0 \wedge \mathcal{A}) \cdot (\mathcal{A} \wedge \mathcal{A})\} \\ &+ \frac{t^4}{T^4} \{(\mathcal{A} \wedge \mathcal{A}) \cdot (\mathcal{A} \wedge \mathcal{A})\} \end{aligned} \quad (6.50)$$

(for which, to the order that we are working, it has been sufficient to take $A_1 = \frac{A}{T}$) and

$$\begin{aligned} \mathbf{E} \cdot \mathbf{E} &= \frac{1}{T^2} \mathcal{A} \cdot \mathcal{A} + \mathcal{A} \cdot (D_0 \wedge \mathbf{B}_0) \\ &+ \frac{1}{3} \mathcal{A} \cdot \{D_0 \wedge (D_0 \wedge \mathcal{A}) + \mathcal{A} \wedge \mathbf{B}_0 + \mathbf{B}_0 \wedge \mathcal{A}\} \\ &+ \frac{1}{6} \mathcal{A} \cdot \{D_0 \wedge (\mathcal{A} \wedge \mathcal{A}) + (D_0 \wedge \mathcal{A}) \wedge \mathcal{A} + \mathcal{A} \wedge (D_0 \wedge \mathcal{A})\} \\ &+ \frac{1}{10} \mathcal{A} \cdot \{\mathcal{A} \wedge (\mathcal{A} \wedge \mathcal{A}) + (\mathcal{A} \wedge \mathcal{A}) \wedge \mathcal{A}\}. \end{aligned} \quad (6.51)$$

Finally using the following identities in (6.50) and (6.51),

$$D_\alpha^{CB} = (\partial_\alpha \delta^{CB} + f^{CAB} A_\alpha^A), \quad (6.52)$$

$$(D \wedge V)_\gamma^C = \epsilon_{\alpha\beta\gamma} D_\alpha^{CB} V_\beta^B = \mathcal{D}_{\gamma\beta}^{CB} V_\beta^B, \quad (6.53)$$

$$\sum_\alpha \epsilon_{\alpha\beta\gamma} \epsilon_{\alpha\mu\nu} = (\delta_{\beta\mu} \delta_{\gamma\nu} - \delta_{\beta\nu} \delta_{\gamma\mu}), \quad (6.54)$$

$$(\epsilon_{\alpha\beta\gamma} \mathcal{D}_{\gamma\mu} \mathcal{A}_\mu)^D = (D_\alpha \mathcal{A}_\beta - D_\beta \mathcal{A}_\alpha)^D, \quad (6.55)$$

$$B_\gamma^V = (\nabla \wedge \mathbf{A} + \mathbf{A} \wedge \mathbf{A})_\gamma^V = \epsilon_{\alpha\beta\gamma} (\partial_\alpha A_\beta + \frac{1}{2} A_\alpha^T A_\beta^U f^{TUV}), \quad (6.56)$$

$$(\mathbf{A} \wedge \mathbf{V})_\gamma^S = (\mathbf{V} \wedge \mathbf{A})_\gamma^S = \frac{1}{2} \epsilon_{\alpha\beta\gamma} V_\alpha^T A_\beta^U f^{TUS}, \quad (6.57)$$

where V is any vector field with both a gauge group and a space-time index, after an integration over the time variable we arrive at the same expression as previously for $W_\tau[\mathbf{A}, \mathbf{A}']$ (6.42). As a final check note that when the initial and final gauge fields are identified $\mathcal{A} = 0$, our expression reduces, as it should, to $-\tau \int d^3\mathbf{x} \mathbf{B}^2 / (2g^2)$, i.e. minus the Euclidean action evaluated for a time-independent potential.

To conclude, we have shown how the analyticity properties of the Schrödinger functional can be used to reconstruct it from a small time (τ) expansion, $1/\tau$ acting as an

infra-red regulator. The next step is to incorporate loop corrections to our analysis. For this task, we have to construct a regulated laplacian in order to “point-split” the ill-defined product of two functional derivatives at the same spatial point so that the Hamiltonian operator has a finite action on our local expansion. For example, Δ acting on $-tr \mathbf{A}^2(\mathbf{x})$ is proportional to $\delta(0)$ which is meaningless. In other words, we have to build a suitable kernel such that the new regulated laplacian respects the symmetries of theory, such as gauge invariance and the underlying geometry of the Hamiltonian operator, and is amenable for calculations. As a result we will inevitably end up with an arbitrariness which is necessary to separate the finite part from the quantities that diverge as we remove the cut-off. In a renormalisable theory, this arbitrariness can be absorbed into (bare) coupling constant, so that the physical quantities will not depend on it. Because of Symanzik’s results [5], we know that the wave functional will be finite as any cut-off is removed.

We have also computed the local expansion of the leading order term in the semi-classical expansion of the Schrödinger functional for Yang-Mills theory using two different approaches, the first by substituting our local expansion directly into the Hamilton-Jacobi equation, the second by computing the on-shell Euclidean action. It turned out that the former approach was far more efficient. The result describes the leading short-time behaviour.

Recently, the Schrödinger functional has been used to define the running coupling constant at a length scale τ in pure Yang-Mills theories which is accessible for calculations on the lattice from perturbative to non-perturbative scales [42]. A continuum small time expansion could be a precious guide for any lattice result.

Chapter 7

Conclusions and Outlook

In general the vacuum wave functional $\Psi[\varphi] = \exp W[\varphi]$ is a non-local object. As we illustrated in chapter 5 for ϕ_{1+1}^4 -theory, $W[\varphi]$ is a sum of connected Euclidean Feynman diagrams in which φ can be interpreted as the source for $\dot{\phi}$ on the boundary. However, in a theory in which the lightest physical particle has non-zero mass, say m_0 , its logarithm is expandable in terms of local functionals if the fields vary slowly on the scale of $1/m_0$. This simplification is the basis of a scheme to solve the eigenvalue problem of the Schrödinger equation for the wave functionals. Let us briefly recall our motivations. In Yang-Mills theory a local expansion of the vacuum functional is justified by the presumed generation of a mass gap. This results in confinement via arguments of dimensional reduction. That is to say, the term of lowest dimension in the large distance expansion of the logarithm of the vacuum functional, leads to a confining area law for the Wilson loop [1]. This commends the local expansion as a tool for studying the large distance behaviour in that theory. To go further so as to obtain physical quantities (e.g. the string tension) we would have to compute more coefficients in the local expansion. On the other hand, we also have discussed in this thesis that this local expansion is suitable to understand physics on all length scales because analyticity arguments show that functionals for arbitrary field configurations can be reconstructed from their local expansion. In principle, this may enable us to extract the light hadron spectrum from the local expansion.

The coefficients of the local expansion are in principle obtained by solving the Schrödinger equation. However, as we demonstrated in the simple case of the free scalar theory (eqns. (2.20) and (2.21)), the Hamiltonian, or more particularly the laplacian, fails to reproduce the correct short distance behaviour. It leads to divergences of increasing order

according to the dimension of the term in the local expansion. This is not surprising as the ultraviolet cut-off contained in the laplacian is a short distance object whereas our local expansion refers to slowly varying fields and in principle could not tell about the ultraviolet behaviour. Our claim, as we explained in section 3.4, was that because of the analyticity properties under complex scaling of the cut-off and the fields we could resum the cut-off dependence of the laplacian and get the correct short distance behaviour, in the same spirit as we did for equation (2.21). In other words, our expectation was that after resumming the divergences that appear by acting with the Hamiltonian on the local expansion and therefore reducing the eigenvalue problem to a set of algebraic equations for its coefficients, they would be finite or could be made finite by the usual renormalisation procedure and perhaps a further field renormalisation according to Symanzik [5].

In chapter 4 we verified in the context of ϕ_{1+1}^4 -theory that our large distance expansion gets the right short distance behaviour as contained in the counterterms of the Hamiltonian. We studied the mass and energy subtraction. The approximation scheme consisted in truncating the series of local functionals to a certain order. Having obtained some exact semi-classical results in which no resummation is involved, we verified that our expansion coefficients agree to within a few percent when the series is truncated to about ten terms. Similar accuracy was found for the mass and energy subtraction. In addition to this, we found a curious simplification that occurs for the Sine-Gordon and Sinh-Gordon models. We verified, up to four fields, that the ratios of the coefficients of the one loop corrections to the coefficients of the local functionals to their tree level values are approximately the same for functionals of the same dimensions. At this stage, it is not clear for us the mechanism responsible for this simplification, if any.

An elegant description of the vacuum functional in terms of Feynman diagrams was presented in chapter 5. The amplitudes were calculated and reproduce the semi-classical results obtained by a direct semi-classical solution of the Schrödinger equation for ϕ_{1+1}^4 -theory.

Within the usual semi-classical solution of ϕ^4 theory, the Schrödinger equation approach brings no novelty. However, Mansfield in [2] suggested a new approach to solve the algebraic equations, as we briefly discussed in section 3.6, which presents two remarkable characteristics. Firstly it can be applied to theories in which mass is generated only

at quantum level and hence that cannot be solved semi-classically within our approach. Secondly it does not rely on the smallness of the coupling constant. In order to develop this approach we will have to improve our computer program shown in appendix B so as to generate a sufficient number of equations. This approach could be useful for studying the spectra of other field theories where the semi-classical approach is not useful, such as Toda field theories in the strong coupling limit.

For Yang-Mills theory an additional technicality occurs. It requires the construction of a suitable laplacian that respects gauge invariance and the underlying geometry of the Hamiltonian operator. Apart from this, the formulation of the eigenvalue problem should be pretty similar to the ϕ^4 -theory. No additional boundary counterterms are needed for Yang-Mills theories as we discussed in section 1.6.

Finally, in chapter 6 we presented some applications of this formalism to the Schrödinger functional for which it is possible to carry out a semi-classical analysis as the time serves as an infrared cut-off. We obtained the leading order short time behaviour of the Yang-Mills-Schrödinger functional within a local expansion in the fields. This preliminary calculation sets the grounds for a more detailed analysis that brings in the quantum corrections. We have also shown how a small time expansion of the Schrödinger functional can be used to reconstruct the Schrödinger functional for arbitrary time based on its analyticity properties.

Appendix A

Analyticity of $(\Delta_s W)[\varphi_s]$

Here we sketch the proof that $(\Delta_{s\epsilon} W)[\varphi_s]$ extends to an analytic function in the complex s plane with the negative real axis removed [2]. Consider the matrix element

$$\langle \varphi | \hat{\pi}(x, t) \hat{\pi}(x', t') | 0 \rangle. \quad (\text{A.1})$$

We soon will take $t = t' = 0$ and then integrate against $\int_{p^2 < 1/s} dp / (2\pi) \exp(ip(x - x'))$, in order to get $(\Delta_s \Psi)[\varphi]$.

In a similar way as we did for the study of the analyticity of the vacuum functional (see chapter 2), it will be helpful to make the φ dependence of $\langle \varphi |$ explicit by defining a representation with the bra $\langle D |$ (D for Dirichlet):

$$\langle \varphi | = \langle D | e^{i \int dx \varphi(x) \hat{\pi}(x)}, \quad (\text{A.2})$$

We also need the identity

$$T(\hat{\pi}(x, t) \hat{\pi}(x', t')) = \frac{\partial^2}{\partial t \partial t'} T(\hat{\varphi}(x, t) \hat{\varphi}(x', t')) - i\delta(x - x')\delta(t - t') \quad (\text{A.3})$$

(Minkowski space). Using the standard relationship between functional integrals and time ordered products, we can express $\langle \varphi | e^{-it_0 \hat{H}} | D \rangle$ as

$$\int \mathcal{D}\tilde{\varphi} e^{iS[\tilde{\varphi}] + \int dx (i\varphi \tilde{\varphi})} \quad (\text{A.4})$$

where we dropped a term coming from a delta function in time. It has no effect in what follows [2] and it can be subtracted by an equal and opposite counterterm in the lagrangian as we have seen in chapter 5. $|D\rangle$ implies Dirichlet boundary conditions $\tilde{\varphi} = 0$ at times 0 and t_0 . Similarly we can write for the time ordered Green's function

$$T\langle \varphi | e^{-it_0 \hat{H}} \hat{\varphi}(x, t) \hat{\varphi}(x', t') | D \rangle = \int \mathcal{D}\tilde{\varphi} e^{iS[\tilde{\varphi}] + \int dx (i\varphi \tilde{\varphi})} \tilde{\varphi}(x, t) \tilde{\varphi}(x', t'). \quad (\text{A.5})$$

Using (A.3), rotating to Euclidean space and taking the limit $t_0 \rightarrow \infty$ yields, for $0 > t \geq t'$,

$$\begin{aligned} \langle \varphi | \hat{\pi}(x, t) \hat{\pi}(x', t') | 0 \rangle = \\ - \int \mathcal{D}\tilde{\varphi} e^{-S_E[\tilde{\varphi}] + \int dx (\varphi \tilde{\varphi})} \left(\dot{\tilde{\varphi}}(x, t) \dot{\tilde{\varphi}}(x', t') - \delta(x - x') \delta(t - t') \right) \end{aligned} \quad (\text{A.6})$$

with $\tilde{\varphi}$ defined on the Euclidean half plane $t \leq 0$ and $\tilde{\varphi}(x, 0) = 0$. To obtain $\langle \varphi | \hat{\pi}(x, 0) \hat{\pi}(x', 0) | 0 \rangle$ we can, for example, take the limit as $t, t' \uparrow 0$ keeping $t > t'$, in which case the δ functions will not contribute [2]. We also rotate the coordinates so that the points $(x, 0)$ and $(x', 0)$ differ by the Euclidean time $\tau = |x - x'|$. Hence (A.6) can be rewritten as

$$\int \mathcal{D}\tilde{\varphi}_\tau e^{-S_{E\tau}[\tilde{\varphi}] + \int dt \varphi \tilde{\varphi}'_\tau} \tilde{\varphi}'_\tau(0, x + \tau) \tilde{\varphi}'_\tau(0, x), \quad (\text{A.7})$$

in which $\tilde{\varphi}_\tau$ is defined for all t ($-\infty < t < \infty$) and $x > 0$, and reinterpreted as the time ordered expectation value of fields which evolve according to a rotated hamiltonian on the half line $x > 0$:

$$T_E \langle 0_r | e^{\int dt \varphi(t) \hat{\varphi}'(0, t)} \hat{\varphi}'(0, x + \tau) \hat{\varphi}'(0, x) | 0_r \rangle \quad (\text{A.8})$$

where $|0_r\rangle$ is the vacuum of the rotated hamiltonian. In order to evaluate (A.8), expand the exponential

$$e^{\int dt \varphi(t) \hat{\varphi}'(0, t)} = \sum_n \frac{1}{n!} \left(\int_{-\infty}^{+\infty} dt \varphi(t) \hat{\varphi}'(0, t) \right)^n \quad (\text{A.9})$$

Suppose

$$t_n > t_{n-1} > \dots > t_p > \tau > t_{p-1} > \dots > t_q > 0 > t_{q-1} > \dots > t_2 > t_1.$$

Then a combinatorial factor cancels the $n!$ and making the Euclidean time dependence explicit enable us to write (A.8) as a sum of terms of the form

$$\begin{aligned} \int_\tau^\infty dt_n \int_\tau^{t_n} dt_{n-1} \dots \int_\tau^{t_{p+1}} dt_p \int_0^\tau dt_{p-1} \dots \int_0^{t_{q+1}} dt_q \int_{-\infty}^0 dt_{q-1} \dots \int_{-\infty}^{t_2} dt_1 \varphi(t_n) \dots \varphi(t_1) \\ \langle 0^r | \hat{\varphi}' e^{-\hat{H}_\tau(t_n - t_{n-1})} \hat{\varphi}' \dots e^{-\hat{H}_\tau(t_p - \tau)} \hat{\varphi}' e^{-\hat{H}_\tau(\tau - t_{p-1})} \hat{\varphi}' \dots \\ e^{-\hat{H}_\tau t_q} \hat{\varphi}' e^{\hat{H}_\tau t_{q-1}} \hat{\varphi}' \dots \hat{\varphi}' e^{-\hat{H}_\tau(t_2 - t_1)} \hat{\varphi}' | 0^r \rangle \end{aligned} \quad (\text{A.10})$$

We fourier transform the sources to evaluate the time integrals

$$\varphi(t_i) = \frac{1}{2\pi} \int dk_i \tilde{\varphi}(k) \exp(ik_i t_i). \quad (\text{A.11})$$

After integrating over x , this gives a delta function conserving the total momentum $\delta(\sum k_i)$ and for t_i with $i < q$ gives insertions of $(\hat{H}_\tau + i \sum k_i)^{-1}$ whereas for $i \geq p$ gives insertions

of $(\hat{H}_r - i \sum k_i)^{-1}$. For example, the t_1 - integral is

$$\int_{-\infty}^{t_2} dt_1 e^{ik_1 t_1} e^{-\hat{H}_r(t_2-t_1)} = \frac{e^{ik_1 t_2}}{(\hat{H}_r + ik_1)}, \quad (\text{A.12})$$

that contributes to the t_2 -integral

$$\int_{-\infty}^{t_3} dt_2 e^{(i(k_1+k_2)+\hat{H}_r)t_2} \hat{\varphi}' \frac{1}{(\hat{H}_r + ik_1)} \hat{\varphi}' |0^\tau \rangle \quad (\text{A.13})$$

where the integral evaluates to $\exp(i(k_1 + k_2) + \hat{H}_r)t_3)/(\hat{H}_r + i(k_1 + k_2))$.

On the other hand, the t_n, t_{n-1} , etc. integrals may be performed by first changing the variables

$$t'_n = t_n - \tau, \quad t'_{n-1} = t_{n-1} - \tau \quad \dots \quad (\text{A.14})$$

and using that $\int_0^a dx \int_0^x dy f(x)g(y) = \int_0^a dy \int_y^a dx f(x)g(y)$ to get

$$\begin{aligned} & (\dots) \langle 0^\tau | \hat{\varphi}' \frac{1}{(\hat{H}_r - ik_n)} \hat{\varphi}' \dots \hat{\varphi}' \frac{1}{(\hat{H}_r - i(k_n + k_{n-1} + \dots + k_p))} \hat{\varphi}' e^{(i(k_n + k_{n-1} + \dots + k_p) - \hat{H}_r)\tau} \times \\ & \times e^{\hat{H}_r \tau} \hat{\varphi}' e^{-\hat{H}_r \tau} \int_0^\tau dt_{p-1} e^{ik_{p-1} t_{p-1}} e^{\hat{H}_r t_{p-1}} \hat{\varphi}' e^{-\hat{H}_r t_{p-1}} \int_0^{t_{p-1}} dt_{p-2} e^{ik_{p-2} t_{p-2}} e^{\hat{H}_r t_{p-2}} \hat{\varphi}' e^{-\hat{H}_r t_{p-2}} \\ & \dots \int_0^{t_{q+1}} dt_q e^{ik_q t_q} e^{\hat{H}_r t_q} \hat{\varphi}' e^{-\hat{H}_r t_q} \hat{\varphi}' \frac{1}{(\hat{H}_r + i \sum_{i=1}^{q-1} k_i)} \hat{\varphi}' \dots \hat{\varphi}' |0^\tau \rangle \quad (\text{A.15}) \end{aligned}$$

The remaining integrals ($t_i, p < i < q$) can be done by inserting a complete base of eigenkets of the Hamiltonian between each operator. This leads to a sum of products of energy denominators of the form $(E_1 - E_2 - i \sum k_j)^{-1}$ multiplied by exponentials of τ of the form $\exp - (E_1 - i \sum k_j)$, so that we have the τ dependence explicit as a sum of integrals over the spectrum of \hat{H}_r :

$$\int dE dk_1 \dots dk_n \tilde{\varphi}(k_1) \dots \tilde{\varphi}(k_n) \delta(\sum k_i) (\rho_0 + \rho_1 e^{ik\tau} + \rho_2 e^{i(k_1+k_2)\tau} + \dots) e^{-E\tau} \quad (\text{A.16})$$

In order to obtain $\Delta_s \Psi[\varphi]$ we integrate against $\int_{p^2 < 1/s} dp / (2\pi) \exp(ip(x-x'))$ to get a sum of terms of the form

$$\int_{p^2 < s^{-1}} \frac{dp}{\pi} \int dE dk_1 \dots dk_n \tilde{\varphi}(k_1) \dots \tilde{\varphi}(k_n) \delta(\sum k_i) \sum \frac{\rho_j(E, k_1, \dots, k_n)}{E - i(p + \sum k_i)} \quad (\text{A.17})$$

Now evaluate for the scaled field $\varphi^s(x) = f(\frac{x}{\sqrt{s}})$ which is, in the momentum space, $\tilde{\varphi}^s(k) = \tilde{f}(k\sqrt{s})\sqrt{s}$. Also, as we want to study the s dependence, let us set $p = q/\sqrt{s}$, and we take $\varphi^s(k)$ to vanish outside $|k| < \kappa \ll 1$. This enable us to scale the k_i integrals to get

$$\int_{q^2 < 1} \frac{dq}{\pi} \int dE dk_1 \dots dk_n \tilde{f}(k_1) \dots \tilde{f}(k_n) \sqrt{s} \delta(\sum k_i) \sum \frac{\rho_j(E, k_1, \dots, k_n)}{\sqrt{s}E - i(q + \sum k_i)} \quad (\text{A.18})$$

The functions ρ_j acquire a dependence on s via the energy denominators that can be written after scaling of k_i as $1/((E_1 - E_2) - i(\sum k)/\sqrt{s})$. Now we take s to be complex to conclude that $(\Delta_s \Psi)[\varphi_s]$ and hence $(\Delta_s W)[\varphi_s]$, since any additional singularities could not cancel between connected and disconnected pieces, extends to an analytical function in the whole complex plane excluding the real negative axis.

Appendix B

Computer Program

In this appendix, we briefly recall the problem of calculating the coefficients of the local expansion of the logarithm of the ϕ_{1+1}^4 theory vacuum functional, W . Then we discuss some of the algorithms that we have used to construct a program in ©MAPLE, which has helped us to obtain some of the results described in chapter 4. Finally, we comment on the efficiency of the program and the software in executing our initial objectives.

B.1 The Problem

The local expansion of W (3.1) satisfies its own form of the Schrödinger equation as we explained in section 3.4. The resulting algebraic equations for the coefficients of the local expansion which we called $I_{j_0\dots j_n} = 0$ (3.22) can then be solved semi-classically, as we illustrated in chapters 3 and 4, and within a new scheme that does not rely on perturbation theory in the coupling [2]. Furthermore, it can be applied to theories which are massless at classical level such as Yang-Mills. In either approach to the solution of the equations, it is desirable to generate both a large number of equations and a large number of terms in each of them. These equations are generated by the Schrödinger equation satisfied by the local expansion. It basically comprises two terms which we call by convenience \mathcal{A} and \mathcal{B} , namely the laplacian

$$\mathcal{A} \equiv \Delta_s W_{local} = \left(\int dx dy \int_{p^2 < 1/s} \frac{dp}{2\pi} e^{ip(x-y)} \frac{\delta}{\delta\varphi(x)} \frac{\delta}{\delta\varphi(y)} \right) W_{local} \quad (\text{B.1})$$

and

$$\mathcal{B} \equiv \int dx \left(\frac{\delta W_{local}}{\delta\varphi(x)} \right)^2. \quad (\text{B.2})$$

The latter generates the $O(\hbar^0)$ terms in (3.22) whereas the former, after applying the resummation operator, gives the λ -dependent terms.

We have elaborated a computer program using ©Maple programming language to calculate the two pieces \mathcal{A} and \mathcal{B} having W_{local} as an input. We were mainly motivated by the sophisticated library that is offered by this software which in principle should make our routines for algebraic computations not too lengthy. It turned out that as the size of the input increased, a few library routines failed to produce the expected results. We also had problems of memory inefficiency and lack of speed with the computers we had available. Roughly speaking, the limit that we reached in obtaining reliable results was with a set of basis vectors up to dimension $D = 6$ and $F = 6$ fields, the number of dimensions corresponding to the number of derivatives. This was useful to some calculations in chapter 4 which allowed us to compute $O(\hbar)$ corrections to some 2-field and 4-fields coefficients in order to perform the energy and mass subtraction.

For example, for $F = 6$ and $D = 8$, our program failed to execute the operations in a reasonable time. The major problem comes from the term \mathcal{B} , which is non-linear. There are 30 basis vectors up to $F = 6$ and $D = 8$. The product $(\delta W_{local}/\delta\varphi)^2$ contains 5885 terms which should be reduced to basis vectors via integration by parts in order to extract the leading order terms of the equations $I_{j_0\dots j_n} = 0$. The laplacian also failed to give reliable results as the dimension became large ($D > 12$). In summary, the algorithms which we present below should be adapted to another programming language (perhaps C^{++}), particularly for the task of solving the problem non-perturbatively according to the scheme proposed in [2].

B.2 The Program

In this program, we have translated a general basis vector

$$\int dx \varphi^{j_0} \dots \varphi^{(n)j_n} \quad (\text{B.3})$$

into a sequence

$$[[0, j_0], [1, j_1], \dots, [n, j_n]]. \quad (\text{B.4})$$

In calculating \mathcal{A} and \mathcal{B} we have used a common set of procedures. Basically, a routine which performs functional differentiations and other routines which act after the opera-

tions encoded in \mathcal{A} and \mathcal{B} are performed, resulting in a sum of terms that might contain reducible elements. The latter are elements that can be transformed into basis-vectors via integration by parts. As we discussed in section 3.3, a linearly independent basis is specified by insisting that the power of the highest derivative be at least two. Thus we create a procedure to read these elements and identify the reducible ones, which will go through another routine that perform the integration by parts.

B.2.1 Root Program for \mathcal{A}

GE is the input functional. $lapl$ initiates the procedure of differentiations. G is the first functional derivative and $D(G)$ is the second. PI is the regularised action of the laplacian on the functional, with momentum cut-off $1/s$. $elen$ consists of a set of routines which are common to \mathcal{B} , which we will explain soon. $Fwtini$ is a subroutine which takes PI through $elena$ in order to transform the reducible elements into basis-vectors. The result is a collection of terms which depend on the cut-off s , which we shall finally re-sum.

```

lapl:= proc(GE)
local
j,aux1,dfxim,result,final,k,PI,RPI,in2,rrr,in3,rrrr,G,inp2,r,inp3,rr,FWT;

fdiffy(f,a,y);

in2[30]:=D(GE);
for rrr from 30 by -1 to 1 do
  in2[rrr-1]:=subs(diff(f(a),a$rrr)=gg[rrr](a),in2[rrr]);
od;

in3[0]:=int(in2[0],a=-infinity..infinity);

for rrrr from 1 to 30 do
  in3[rrrr]:=subs(gg[rrrr](y)=diff(f(y),y$rrrr),in3[rrrr-1]);
od;

```

```
fdiffy(f,y,x);
```

```
G:=in3[30];
```

```
inp2[35]:=expand(D(G)*exp(I*p*(x-y)));
```

```
for r from 35 by -1 to 1 do
```

```
  inp2[r-1]:=subs(diff(f(y),y$r)=g[r](y),inp2[r]);
```

```
od;
```

```
inp3[0]:=int(inp2[0],y=-infinity..infinity);
```

```
for rr from 1 to 35 do
```

```
  inp3[rr]:=subs(g[rr](x)=diff(f(x),x$rr),inp3[rr-1]);
```

```
od;
```

```
PI:=expand(int(inp3[35],p=-s^(-1/2)..s^(-1/2)));
```

```
FWT:=fwtini(PI);
```

```
RETURN(FWT);
```

```
elena:=proc(QQ)
```

```
  local QQ1,EE,RR,WW,AA,FINAL;
```

```
  WW:=master(expand(QQ),30);
```

```
  EE:=compare(WW);
```

```
  RR:=masa1((op(1,EE)));
```

```
  AA:=mega(RR);
```

```
  FINAL:=AA+masa1(op(2,EE));
```

```
  RETURN(FINAL);
```

```
  RETURN(WW);
```

```
end;
```

```
fwtini:=proc(inp1)
```

```
  local l,var1,var2,var3,var4,var5,var6,var7,var8,i,inp11,var22;
```

```

l:=0;
var7[0]:=0;
elen(0):=0;
inp1:=sorte(inp1,40);
var1:=subs(s=1/LL^2,inp1);
var2:=subs(1/sqrt(Pi)=1,var1);
var22:=simplify(subs(x=t,var2));
var3:=subs(csgn(conjugate(LL))=1,sorte(collect(var22,LL),40));
for i from 0 to nops(inp1)-1 do
  l:=l+1;
  var4[i]:=coeff(var3,LL^(2*i+1));
  var5[i]:=elena(sorte(var4[i],40));
  var6[i]:=var5[i]*1/s^((2*i+1)/2);
  var7[l]:=var7[l-1]+var6[i];
  var8[l]:=var8[l-1],var5[i];
od;
RETURN(var7[l]);
end;

```

B.2.2 Root Program for B

The root program is called *elen*. It commands the product of the two functional derivatives of W and send the result through the auxiliary routines so to turn all the elements into an irreducible form.

```

elen:=proc(HHH)
local QQ1,EE,RR,AA,FINAL,QQ,n,sel1,sel2;
fdiff(f,x,40);
VC:=expand(D(HHH));
imnp2[35]:=VC;
for r from 35 by -1 to 1 do
  imnp2[r-1]:=subs(diff(f(x),x$r)=gg[r](x),imnp2[r]);

```

```

od;

imnp3[0]:=expand((int(imnp2[0],x=-infinity..infinity))^2);

for rr from 1 to 35 do
  imnp3[rr]:=subs(gg[rr](t)=diff(f(t),t$rr),imnp3[rr-1]);
od;

QQ:=sorte(imnp3[35],40);
WW:=master(QQ,40);
EE:=compare(WW);
RR:=masa1(op(1,EE));
AA:=mega(RR,40);
FINAL:=AA+masa1(op(2,EE));
sel1:=master(FINAL,40);
RETURN(sel1);
end;

```

B.2.3 Auxiliary Routines

We present the auxiliary routines for calculating \mathcal{A} and \mathcal{B} . *fdiff* defines the functional differentiations. *sorte* organizes an expression in increasing order of the derivatives. *master* is a routine to translate (B.3) into (B.4) with the help of the subroutines *faf*, which reads the number of derivatives, and *pow* which reads the power. *compare* reads an input and separates it into two sets: basis-vectors and non-basis-vectors. *masa1* is the inverse of *master*. Finally *mega* reduces non-basis-vectors to basis vectors via a kind of integration by parts. We illustrate the results of the program and a few routines in the end.

- *fdiff*

```

fdiff:=proc(F,X,n)
  local i;
  D(x):=0;

```

```

for i from 1 to n do
  D(diff(F(X),X$i)):=Dirac(i,X-t);
  D(F(X)):=Dirac(X-t);
  D(z[i]):=0;
od;
RETURN(FDifferentiation_defined);
end;

```

- sorte

```

sorte:=proc(inp1,n)
local l,i;
l:=0;
var2[0]:=f(t);
for i from 1 to n do
l:=l+1;
var2[l]:=var2[l-1],diff(f(t),t$i);
od;
var1:=sort(inp1,[var2[l]]);
RETURN(var1);
end;

```

- master

```

master:=proc(inp1,n)
local inp2,i1;
inp2:=NULL;
if type(inp1,'+') then
  for i1 to nops(inp1) do
    inp2:=inp2,[pow(op(i1,inp1),n)];
  od;
elif type(inp1,'*') then inp2:=[pow(inp1,n)];
elif type(inp1,**') then
inp2:=[faff(op(1,inp1),n),op(2,inp1)];

```

```

elif type(inp1,'numeric') then inp2:=[[inp1,'number']];
elif type(inp1,'function') then inp2:=[faff(inp1,n),1];
else ERROR('Wrong format for us!');
fi;
RETURN([inp2]);
end;

```

- faff

```

faff:=proc(q,n)
local inp1,inp2,inp3,l,i;
l:=0;
inp2[0]:=NULL;
for i from 1 to n do
l:=l+1;
if q=diff(f(t),t$i) then
inp1[i]:=i;
elif q=z[i] then inp1[i]:=z[i];
else inp1[i]:=NULL;
fi;
inp2[l]:=inp2[l-1],inp1[i];
od;
if inp2[n]=NULL and q=f(t) then inp3:=0
else inp3:=inp2[n] fi;
RETURN(inp3);
end;

```

- pow

```

pow:=proc(q,n)
local inp1,inp2,inp3,ind2,i,j,l,k;
l:=0;
k:=0;

```

```

inp2[0]:=NULL;
if type(op(1,q),numeric) and nops(q)<>1 then
  if nops(q)=2 and type(op(2,q),'**') then
    inp2[nops(q)-1]:=[faff(op(1,op(2,q)),n),op(2,op(2,q))]
  elif type((q/(op(1,q))),'*') then
    for i from 2 to nops(q) do
      k:=k+1;
      if type(op(i,q),'**') then
        inp1[i]:=(faff(op(1,op(i,q)),n),op(2,op(i,q)));
      else inp1[i]:=(faff(op(i,q),n),1);
      fi;
      inp2[k]:=inp2[k-1],[inp1[i]];
    od;
  else inp2[nops(q)-1]:=[faff(op(2,q),n),1];
  fi;
inp3:=( [op(1,q),'number'],inp2[nops(q)-1] );
elif nops(q)=1 and type(q,numeric) then
inp3:=( [q,'number'] );
else
  if type(q,'^') then inp2[nops(q)]:=[faff(op(1,q),n),op(2,q)]
  elif type(q,'*') then
    for j from 1 to nops(q) do
      l:=l+1;
      if type(op(j,q),'**') then
        inp1[j]:=(faff(op(1,op(j,q)),n),op(2,op(j,q)));
      else inp1[j]:=(faff(op(j,q),n),1);
      fi;
      inp2[l]:=inp2[l-1],[inp1[j]];
    od;
  else inp2[nops(q)]:=[faff(q,n),1];
  fi;
inp3:=inp2[nops(q)]

```



```

fi;
RETURN(inp3);
end;

```

- compare

```

compare:=proc(inp1)
local var0,var1,var2,var3,var4,var5,var11,i1,l;
l:=0;
var3[0]:=NULL;
var11[0]:=NULL;
if nops(inp1)=1 and nops(op(1,inp1))=1 and nops(op(1,op(1,inp1)))=2
and op(2,op(1,op(1,inp1)))=number then
var4:='Number';
var5:=op(1,op(1,op(1,inp1)));
elif nops(inp1)=1 then
if nops(op(1,inp1))=1 and type(op(2,op(1,op(1,inp1))),'numeric')
then if op(2,op(1,op(1,inp1)))=1 and
type(op(1,op(1,op(1,inp1))),'numeric') then
var4:='It is 1';
var5:=op(1,inp1);
else var4:='It is not 1';
var5:=op(1,inp1);
fi;
elif nops(op(1,inp1))>1 and op(2,op(nops(op(1,inp1)),op(1,inp1)))=1
and type(op(1,op(nops(op(1,inp1)),op(1,inp1))),'numeric') then
var4:='It is 1';
var5:=op(1,inp1);
else var4:='It is not 1';
var5:=op(1,inp1);
fi;
elif nops(inp1)>1 then
for i1 from 1 to nops(inp1) do
l:=l+1;

```

```

if nops(op(i1,inp1))=1 and nops(op(1,op(i1,inp1)))=2 and
op(2,op(1,op(i1,inp1)))=number then
    var2[i1]:='Number';
    var1[i1]:=op(i1,inp1);
elif nops(op(i1,inp1))=1 and nops(op(1,op(i1,inp1)))=2 and
type(op(2,op(1,op(i1,inp1))), 'numeric')
then
    if op(2,op(1,op(i1,inp1)))=1 and
type(op(1,op(1,op(i1,inp1))), 'numeric') then
        var2[i1]:='It is 1';
var1[i1]:=op(i1,inp1);
    else var2[i1]:='It is not 1';
        var1[i1]:=op(i1,inp1);
    fi;
elif op(2,op(nops(op(i1,inp1)),op(i1,inp1)))=1 and
type(op(1,op(nops(op(i1,inp1)),op(i1,inp1))), 'numeric') then
    var2[i1]:='It is 1';
    var1[i1]:=op(i1,inp1);
else var2[i1]:='It is not 1';
    var1[i1]:=op(i1,inp1)
fi;
var3[1]:=var3[l-1],var2[i1];
var11[1]:=var11[l-1],var1[i1];
od;
var4:=var3[1];
var5:=var11[1];
fi;

sas:=[[var4],[var5]];

l1:=0;
k1:=0;

```

```

var13[0]:=NULL;
var14[0]:=NULL;
var11:=op(1,sas);
var12:=op(2,sas);
for i11 from 1 to nops(var11) do
  if op(i11,var11)='It is 1' then
    l1:=l1+1;
    var13[l1]:=var13[l1-1],op(i11,var12);
  elif op(i11,var11)='It is not 1' then
    k1:=k1+1;
    var14[k1]:=var14[k1-1],op(i11,var12);
  fi;
od;
var15:=var13[l1];
var16:=var14[k1];
var17:=[[var15],[var16]];
RETURN(var17);
end;

```

- masal

```

masal:=proc(inp1)
local var0,var1,i0,l;
l:=0;
var1[0]:=0;
if nops(inp1)<>1 then
  for i0`from 1 to nops(inp1) do
    l:=l+1;
    var1[l]:=var1[l-1]+masa(op(i0,inp1));
  od;
  var0:=NULL;
elif nops(inp1)=1 then
  var0:=masa(op(1,inp1));

```

```
var1[0]:=NULL;
fi;
RETURN(var0,var1[1]);
end;
dif:=proc(inp1,n)
local var1;
if n=0 then var1:=inp1;
elif n<>0 and type(n,numeric) then
    var1:=diff(inp1,t$n);
elif type(n,indexed) then
    var1:=n;
fi;
RETURN(var1);
end;

masa:=proc(inp1)
local var1;
l:=0;
var1[1]:=1;
if nops(inp1)=1 then
    if op(2,op(1,inp1))=number then var0:=op(1,op(1,inp1));
    else var0:=dif(f(t),op(1,op(1,inp1)))^op(2,op(1,inp1));
    fi;
    var1[1]:=NULL;
elif nops(inp1)<>1 and op(2,op(1,inp1))=number then
    for i from 2 to nops(inp1) do
        l:=l+1;
        var1[l]:=op(1,op(1,inp1));
        var1[l+1]:=var1[l]*dif(f(t),op(1,op(i,inp1)))^op(2,op(i,inp1));
    od;
var0:=NULL;
```

```

elif nops(inp1)<>1 and type(op(2,op(1,inp1)),numeric) then
  for i from 1 to nops(inp1) do
    l:=l+1;
    var1[l+1]:=var1[l]*dif(f(t),op(1,op(i,inp1)))^op(2,op(i,inp1));
  od;
var0:=NULL;
fi;
RETURN(var0,var1[l+1]);
end;

```

- mega

```

mega:=proc(A,n)
local q,p,up,uq,var1,var2,l1,var3,var00,T2,l,var11,T3,T,B;
#A:="nbvs";
B:=A;
with(student);
l1:=0;
var3[0]:=0;
while B<>0 do
  if type(B,'+') then
    T:=op(1,B);
  else T:=B;
  fi;
  TM:=op(1,master(T,n));

# with(student);
l:=0;
var2[0]:=NULL;
q:=TM[nops(TM)][1];
p:=TM[nops(TM)-1][1];
uq:=TM[nops(TM)][2];
up:=TM[nops(TM)-1][2];

```

```

if q=p+1 then
  var00:=-diff(product('op(j,T)', 'j'=1..(nops(T)-2)),t)*
  diff(f(t),t$P)^(up+1)/(up+1);
  var11:=sorte(expand(var00),n);
  l1:=l1+1;
var3[l1]:=var3[l1-1]+var11;
  B:=B-T;
else
  T2:=intparts(Int(T,t),product(op(j,T),j=1..(nops(T)-1)))-
  op(1,intparts(Int(T,t),product(op(j,T),j=1..(nops(T)-1))));
  T3:=-sorte(expand(sorte(op(1,-T2),10),n);
  T4:=compare(master(T3,n));
# gives nbv and bv separatedly
  if op(2,T4)<>NULL then
    l1:=l1+1;
    var3[l1]:=var3[l1-1]+masa1(op(2,T4));
    fi;
    T5:=masa1(op(1,T4));
  B:=B-T+T5;
  fi;
od;
RETURN(var3[l1]);
end;

```

B.3 Examples

Suppose that we have

$$A := z_1 f(x)^2 + z_2 \left(\frac{\partial}{\partial x} f(x) \right)^2 + z_3 f(x)^4 + z_4 f(x)^2 \left(\frac{\partial}{\partial x} f(x) \right)^2 \quad (\text{B.5})$$

To execute \mathcal{B} , we write

```
B:=elen(A);
```

to get

$$\begin{aligned}
B := & 64 z_3 z_4 f(t)^4 \left(\frac{\partial}{\partial t} f(t) \right)^2 - 4 z_4^2 f(t)^2 \left(\frac{\partial}{\partial t} f(t) \right)^4 \\
& + 48 z_2 z_3 f(t)^2 \left(\frac{\partial}{\partial t} f(t) \right)^2 + 16 z_1 z_4 f(t)^2 \left(\frac{\partial}{\partial t} f(t) \right)^2 \\
& - \frac{8}{3} z_2 z_4 \left(\frac{\partial}{\partial t} f(t) \right)^4 + 8 z_1 z_2 \left(\frac{\partial}{\partial t} f(t) \right)^2 + 16 z_3^2 f(t)^6 \\
& + 4 z_4^2 f(t)^4 \left(\frac{\partial^2}{\partial t^2} f(t) \right)^2 + 16 z_1 z_3 f(t)^4 + 8 z_2 z_4 f(t)^2 \left(\frac{\partial^2}{\partial t^2} f(t) \right)^2 \\
& + 4 z_1^2 f(t)^2 + 4 z_2^2 \left(\frac{\partial^2}{\partial t^2} f(t) \right)^2
\end{aligned}$$

and to execute \mathcal{A} ,

$C := \text{lapl}(A);$

to get

$$C := \frac{4 z_4 \left(\frac{\partial}{\partial t} f(t) \right)^2 + 24 z_3 f(t)^2 + 4 z_1}{\sqrt{s}} + \frac{\frac{4}{3} z_4 f(t)^2 + \frac{4}{3} z_2}{s^{3/2}} \quad (\text{B.6})$$

Finally let us illustrate how *Mega* works. It reduces a set of non-basis vectors to basis vectors via a series of integration by parts, that is

$\text{NBV} := z[1]*f(t)^3*\text{diff}(f(t),t,t)+$
 $z[2]*f(t)*\text{diff}(f(t),t,t,t,t)+z[3]*f(t)^2*\text{diff}(f(t),t)*\text{diff}(f(t),t,t,t);$

$\text{NBV} :=$

$$z_1 f(t)^3 \left(\frac{\partial^2}{\partial t^2} f(t) \right) + z_2 f(t) \left(\frac{\partial^4}{\partial t^4} f(t) \right) + z_3 f(t)^2 \left(\frac{\partial}{\partial t} f(t) \right) \left(\frac{\partial^3}{\partial t^3} f(t) \right)$$

$\text{BV} := \text{mega}(\text{NBV});$

$$\begin{aligned}
\text{BV} := & -3 z_1 f(t)^2 \left(\frac{\partial}{\partial t} f(t) \right)^2 - z_3 f(t)^2 \left(\frac{\partial^2}{\partial t^2} f(t) \right)^2 + z_2 \left(\frac{\partial^2}{\partial t^2} f(t) \right)^2 \\
& + \frac{2}{3} z_3 \left(\frac{\partial}{\partial t} f(t) \right)^4
\end{aligned}$$

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