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Linear and nonlinear field transformations and their application in the variational approach to nonperturbative quantum field theory

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LINEAR AND NONLINEAR FIELD TRANSFORMATIONS AND THEIR APPLICATION IN THE VARIATIONAL APPROACH TO NONPERTURBATIVE QUANTUM FIELD THEORY

by

RODRIGO IBAÑEZ MEIER

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE DOCTOR OF PHILOSOPHY

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Abstract

Linear and Nonlinear Field Transformations and their Application in the
Variational Approach to Nonperturbative Quantum Field Theory

by

Rodrigo Ibañez Meier

The present work concerns nonperturbative variational studies of the effective potential
beyond the Gaussian effective potential (GEP) approximation. In the Hamiltonian for-
malism, we study the method of non-linear canonical transformations (NLCT) which al-
 lows one to perform variational calculations with non-Gaussian trial states, constructed
by nonlinear unitary transformations acting on Gaussian states. We consider in detail a
particular transformation that leads to qualitative as well as quantitative improvement
over the Gaussian approximation. In particular we obtain a non-trivial correction to
the Gaussian mass renormalization. For a general NLCT state, we present formulas
for the expectation value of the $O(N)$-symmetric $\lambda(\phi^2)^2$ Hamiltonian, and also for the
one-particle NLCT state energy.

We also report on the development of a manifestly covariant formulation, based
on the Euclidian path integral, to construct lower-bound approximations to $\Gamma_{1P}$, the
generating functional of one-particle-irreducible Green's functions. In the Gaussian
approximation the formalism leads to the Gaussian effective action (GEA), as a natural
variational bound to $\Gamma_{1P}$. We obtain, non-trivially, the proper vertex functions at
non-zero momenta, and non-zero values of the classical field. In general, the formalism
allows improvement beyond the Gaussian approach, by applying nonlinear measure-
preserving field transformations to the path integral. We apply this method to the $O(N)$-symmetric $\lambda(\phi^2)^2$ theory. In 4 dimensions, we consider two applications of the GEA. First, we consider the $N = 1 \lambda\phi^4$ theory, whose renormalized GEA seems to suggest that the theory undergoes SSB, but has noninteracting particles in its SSB phase. Second, we study the Higgs mechanism in scalar quantum electrodynamics (i.e., $O(2) \lambda\phi^4$ coupled to a $U(1)$ gauge field) in a general covariant gauge. In our variational scheme we can optimize the gauge parameter, leading to the Landau gauge as the optimal gauge. We derive optimization equations for the GEA and obtain the renormalized effective potential explicitly.
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To my wife Amy and son Danny I give my deepest thanks for their love and support, and all the happiness they have brought into my life.

This thesis is dedicated to the loving memory of my brother Hugo and niece Claudia.
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Chapter 1  Introduction

1.1  The Standard Model and the Higgs Mechanism

The Standard Model (SM) is widely regarded as the model of the known interactions between the elementary particles except for gravity. Encompassing the strong, weak, and electromagnetic forces, the model is based on the gauge group \(SU(3) \times SU(2) \times U(1)\). As a quantum field theory the Standard Model has been successful in those regimes where the coupling constants of the different interactions allow for the solution of the model in terms of well-behaved perturbative expansions. This is certainly the case in quantum electrodynamics, where the coupling constant is small. In quantum chromodynamics, the \(SU(3)\) sector of the model that describes the strong interactions, the relevant coupling constant becomes small only at high energies where perturbative predictions have been successfully supported by experimental data [1]. Much of the interesting physics, however, happens at low energies, where the quark and gluon fields lead to the bound states which constitute the particles of the hadron spectrum. In this regime, where the coupling constant is relatively large, nonperturbative effects become critical. As a result, while a great deal has been learned from the group structure of the model, much of the dynamics of QCD bound states has remained elusive to standard perturbative methods.

A second aspect of the Standard model which is not fully understood is how the elementary particles and massive gauge particles get their masses. As a model built on the gauge symmetry principle, the Lagrangian of the SM is gauge invariant. The addition of any mass terms by hand into the SM Lagrangian would destroy this gauge invariance.
Apparently, the problem of mass generation is solved by the Higgs mechanism, which consists of introducing dynamical self-interacting scalar fields into the theory, that couple to both the electroweak gauge fields and the fermion fields. The mechanism explains how the Lagrangian and Hamiltonian of the theory indeed remain gauge invariant while the gauge symmetry of the vacuum is “spontaneously” broken, leading to masses for the W and Z vector bosons, and to masses for the leptons and quarks [2]. In the vacuum state, one of the scalar fields becomes the matter field for the Higgs boson, and all the remaining scalar fields that would otherwise lead to massless Goldstone bosons disappear, or get “eaten” by the gauge bosons which become massive.

A nice model that illustrates the classical features of the Higgs mechanism is the U(1)-Higgs model, also known as “scalar electrodynamics”. The theory is given by the Lagrangian density

\[ \mathcal{L} = D_\mu \phi^* D^\mu \phi - \mu^2 \phi^* \phi - 4\lambda (\phi^* \phi)^2 - \frac{1}{4} F_{\mu \nu} F^{\mu \nu} \]  

(1.1)

where the covariant derivative \( D_\mu = \partial_\mu - i e A_\mu \). The Lagrangian is invariant under a local U(1) gauge transformation \( \phi(x) \rightarrow e^{i \alpha(x)} \phi(x) \) where the gauge field transforms as \( A_\mu \rightarrow A_\mu + \frac{1}{e} \partial_\mu \alpha \). In the absence of the gauge field the Lagrangian would be just that of the \( O(2) \)-symmetric \( \lambda (\phi^2)^2 \) theory (see Eq. (1.7) below), as one sees by writing the complex scalar field as \( \phi = (\phi_1 + i \phi_2)/\sqrt{2} \). The classical potential

\[ V = \mu^2 \phi^* \phi + 4\lambda (\phi^* \phi)^2 = \frac{1}{2} \mu^2 (\phi_1^2 + \phi_2^2) + \lambda (\phi_1^2 + \phi_2^2)^2, \]

(1.2)

for \( \mu^2 < 0 \) and \( \lambda > 0 \), exhibits a spontaneously symmetry broken (SSB) phase with a circle of minima in the \( \phi_1, \phi_2 \) plane of radius \( v = \frac{1}{2} \sqrt{-\mu^2/\lambda} \), as shown in Fig. 1.1. By
Fig. 1.1. The classical potential $V(\phi)$ (see Eq. (1.2)) for $\mu^2 < 0$ and $\lambda > 0$. The potential has a circle of minima of radius $v = \frac{1}{2} \sqrt{-\mu^2/\lambda}$. 
making a change of variables, one can write the complex field $\phi$ in polar coordinates:

$$
\phi(x) = \frac{1}{\sqrt{2}} [v + h(x)] e^{i\theta(x)/v} 
$$

(1.3)

The Lagrangian density thus becomes a function of the new fields $h$ and $\theta$. However, one can “gauge away” and eliminate the $\theta$ field by performing the following gauge transformation:

$$
A_\mu \rightarrow A_\mu + \frac{1}{e v} \partial_\mu \theta.
$$

(1.4)

Finally, substituting back into $\mathcal{L}$, one obtains:

$$
\mathcal{L} = \frac{1}{2} (\partial_\mu h)^2 - 4\lambda v^2 h^2 + \frac{1}{2} e^2 v^2 A_\mu^2 - 4\lambda v h^3 - \lambda h^4 
+ \frac{1}{2} e^2 A_\mu^2 h^2 + v e^2 A_\mu^2 h - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}.
$$

(1.5)

The Lagrangian in terms of the new fields, depends only on $h$ and $A_\mu$. In the SSB phase both the $A_\mu$ and $h$ fields become massive, and their masses can be read off from the coefficients of their respective quadratic terms in the Lagrangian, i.e.,

$$
m_{\text{vector}}^2 = e^2 v^2 \quad m_h^2 = 8\lambda v^2
$$

(1.6)

The new $h$ field is called the Higgs field. The $\theta$ field, which disappears by virtue of (1.4), would have been a massless field, corresponding to a Goldstone boson. Even though the Goldstone field disappears, the total number of degrees of freedom is conserved. Effectively, one degree of freedom from the original complex scalar field is transferred to the vector field, since a massive vector field has three polarization states, whereas a massless vector field has only two, transverse polarizations.

The Higgs mechanism is well understood at the level of classical field theory. In quantum field theory, however, it has mostly been pursued by essentially perturbative
methods, with no reliable predictions for the Higgs mass. As we have seen, the mechanism hinges on SSB in the scalar sector, which is typically a generalization of $\lambda \phi^4$ (e.g., $O(4) \mathcal{L}(\phi^2)^2$ in the minimal Standard Model). (Higher powers of $\phi$ would give a non-renormalizable theory, at least in perturbation theory.) However, even the existence of a renormalized non-trivially interacting $\lambda \phi^4$ quantum field theory has been controversial [3], suggesting that the usual description of the Higgs mechanism is inadequate or perhaps totally wrong. This is why the study of $\lambda \phi^4$ is of considerable importance. More generally, we are also interested in the $O(N)$-symmetric generalization of $\lambda \phi^4$, which is the $O(N)$-symmetric $\lambda (\phi^2)^2$ theory given by the Lagrangian density:

$$\mathcal{L} = \frac{1}{2} \left( \partial_{\mu} \phi^a \partial^{\mu} \phi^a - m_B^2 \phi^a \phi^a \right) - \lambda_B \int_x (\phi^a \phi^a)^2 ,$$

where $a$ is summed over $1, \ldots, N$.

It would seem that much of the fundamental structure of quantum field theory is simply inaccessible to perturbation theory. Consequently, nonperturbative methods have been the subject of much research in an attempt to fill this void. Examples of such nonperturbative methods are lattice-based Monte-Carlo simulations, the $1/N$ expansion, lattice calculations, and the variational approach.

### 1.2 The Effective Potential

The effective potential is an important tool in the study of spontaneous symmetry breaking (SSB), the crucial ingredient of the Higgs mechanism. The concept was studied by Schwinger [4], and first applied to the study of SSB by Goldstone, Salam, and Weinberg [5], and by Jona-Lasinio [6]. Its physical meaning and formulation in canonical quantization was discovered by Symanzik [7]. The computation of the effective potential
in the one-loop approximation was introduced by Coleman and Weinberg [8], and a functional method to carry out this approximation to higher orders was introduced by Jackiw [9].

The effective potential describes how the energy density of a given theory changes as function of the classical field, which is the expectation value of the field operator \( \phi(x) \). In Symanzik's definition [7], the potential is obtained by minimizing the expectation value of the Hamiltonian over all normalizable physical states in which the expectation value of the field is equal to a given constant "classical field" \( \varphi_c \), i.e.,

\[
V_{\text{eff}}(\varphi_c) = \min_{\Psi} \langle \Psi | H | \Psi \rangle
\]

subject to the constraints

\[
\langle \Psi | \Psi \rangle = 1, \quad \varphi_c = \langle \Psi | \phi | \Psi \rangle.
\]

The minimum of \( V_{\text{eff}} \) is the ground-state energy. The effective potential can also be derived from the path-integral formalism. In that case it is given (up to a negative volume factor) by the Legendre transform of \( W \), the generating functional of connected Greens functions, evaluated at constant classical fields. More precisely, the path integral, or generating functional for the Green's functions (in the Euclidian formalism) is given by:

\[
Z[j] = \int D\phi \ e^{-S[\phi] + \int d^4x j(x)\phi(x)}.
\]

The generating functional for the connected Green's functions is given by

\[
W[j] = -\log Z[j].
\]
The effective action (up to a conventional minus sign), is then given by the Legendre transform of $W$:

$$
\Gamma_{\text{eff}}[\varphi_c] = \int d^d x \ j(x) \varphi_c(x) - W[j],
$$

where

$$
\varphi_c(x) = \frac{\delta W[j]}{\delta j(x)} \quad (1.13)
$$

$$
= Z^{-1}[j] \int D\phi \ \phi \ e^{-S[\phi] + \int d^d x \ j(x)\phi(x)},
$$

and

$$
j(x) = \frac{\delta \Gamma_{\text{eff}}[\varphi_c]}{\delta \varphi_c(x)}. \quad (1.15)
$$

The effective potential is then obtained by evaluating $\Gamma[\varphi_c]$ at constant classical fields:

$$
V_{\text{eff}} = -V^{-1}[\phi]_{\varphi_c(x)=\varphi_c}. \quad (1.16)
$$

The effective potential, in Symanzik's definition, is by construction a convex function, and in the symmetric phase the minimum of the potential, corresponding to the vacuum energy, occurs at $\varphi_c = 0$. In the SSB phase the potential is flat at the bottom between the SSB vacua $-\phi_v$ and $+\phi_v$. (See Fig. 1.2.) This is a consequence of the fact that in the SSB phase, any linear combination of the two possible vacua which has a classical field lying between $-\phi_v$ and $+\phi_v$ is also, formally, a ground state of the Hamiltonian, and therefore has the same energy. Thus the potential being flat at the bottom, because of the superposition principle, loses much of the dynamical information that one normally associates, for example, with classical potentials, where forces acting on particles are simply given by the (negative) gradient of the potential. In the symmetric phase, the effective potential derived from the covariant formalism and the one given
Fig. 1.2. The classical potential $V(\varphi_c)$ (solid line) for the case of SSB, and the corresponding effective potential (dashed line). The effective potential is flat at the bottom between the SSB vacua $-\varphi_v$ and $+\varphi_v$. 
by Symanzik’s definition are the same. However, in the SSB phase one must be careful: At the SSB vacuum one would expect a non-zero value for the expectation value of the field. Equation (1.15) implies that the SSB vacuum must exist in the absence of the source \( j(x) \). However this makes the integrand in (1.14) an odd function of \( \phi \), which apparently results in a zero classical field. The situation is clarified by considering the limit of the RHS of equation (1.14) as \( j(x) = \epsilon \) goes to zero from the left and from the right. As \( \epsilon \) goes to zero from the left (right), the potential in fact approaches \(-\phi_v \) (\(+\phi_v \)) from the left (right), and the region in between the two minima is undefined, because (1.15) has no real solution [10]. The way one usually proceeds is to connect the potential between these two minima by a straight line, in a way similar to the Maxwell construction in thermodynamics. The resulting effective potential then coincides with that obtained from Symanzik’s definition.

As we have seen, the effective potential results from the minimization of wavefunctions whose expectation value is \( \varphi_c \), but which are not necessarily “localized” around \( \varphi_c \) in any sense. As pointed out by Stevenson [11], this results in a potential that can give a misleading impression of the underlying physics. For example, in quantum mechanics, a theory whose classical potential is well-shaped but which tends to a finite value at infinity has an effective potential which is actually flat everywhere, suggesting that the particle is free to wander around, whereas in fact it will be localized around the potential well. Another example is that of a theory with an enormous double-well shaped classical potential. The effective potential being flat at its bottom would suggest that the particle is free to transit between the wells, whereas in fact the particle is exceedingly unlikely to be found in this region. Motivated in part by this, Stevenson proposed
to restrict Symanzik’s definition of the effective potential to Gaussian wavefunctions, which are centered in a real sense about \( \varphi_c \) \([11,12]\), resulting in the Gaussian effective potential (GEP).

### 1.3 The Gaussian Effective Potential

Variational methods using Gaussian states have a long history (see \([12-16]\) and references therein). The GEP is a variational approximation to the effective potential that employs a normalized free-field vacuum state \( |\Psi\rangle \) centered at \( \varphi_c \), and with variable mass \( \Omega \), as a trial ground state:

\[
\bar{V}_G(\varphi_c) = \min\limits_{\Omega} V_G(\varphi_c; \Omega)
\]

(1.17)

with

\[
V_G(\varphi_c; \Omega) \equiv \langle \Psi_G | H | \Psi_G \rangle.
\]

(1.18)

This nonperturbative approximation is known to contain the one loop and leading-order \( 1/N \) results as special limiting cases.

For \( \lambda_B \varphi^4 \), evaluating the expectation value of \( H \), and performing the optimization with respect to \( \Omega \), one obtains \([12]\):

\[
\bar{V}_G = I_1 + \frac{1}{2} m_B^2 \varphi_c^2 + \lambda_B \varphi_c^4 + \frac{1}{2} (m_B^2 - \bar{\Omega}^2) I_0 + 6 \lambda_B I_0 \varphi_c^2 + 3 \lambda_B I_0^2,
\]

(1.19)

where \( \bar{\Omega} \) satisfies the equation

\[
\bar{\Omega}^2 = m_B^2 + 12 \lambda_B \left[ I_0(\bar{\Omega}) + \varphi_c^2 \right].
\]

(1.20)

The integrals \( I_n \) are defined by \((\nu = \text{no. of space dimensions})\):

\[
I_n(\Omega) \equiv \int \frac{d^\nu k}{(2\pi)^\nu 2\omega_k} (\omega_k^2)^n, \quad \omega_k^2 \equiv k^2 + \Omega^2.
\]

(1.21)
In $\nu > 0$ dimensions the integrals $I_1$ and $I_0$ are divergent, but the GEP can be renormalized by eliminating the bare parameters $m_B$ and $\lambda_B$ in favor of two new parameters, $m_R$ and $\lambda_R$, defined in terms of derivatives of $V_G$ at the origin [14,12].

In $0 + 1$ dimensions the 'integrals' $I_1$ and $I_0$ reduce to

$$I_1 = \frac{\Omega}{2}, \quad I_0 = \frac{1}{2\Omega},$$

(1.22)

and the problem reduces to a problem in ordinary quantum mechanics (QM), where one has a lot of intuition and where exact, or very accurate numerical results are readily available.

We review the QM case in detail because it will provide an indication of the extent to which the methods developed in this thesis improve upon the GEP approximation.

Even though the bare parameters are finite in $0 + 1$ dimensions, it is convenient to introduce a "renormalized mass" $m_R$ and a dimensionless coupling constant, $\hat{\lambda}$ through the equations [12]:

$$m_B^2 = m_R^2[1 - 6\hat{\lambda}],$$

$$\lambda_B = \hat{\lambda} m_R^3.$$  \hspace{1cm} (1.23)

For the anharmonic oscillator case ($m_B^2 > 0$, i.e., $\hat{\lambda} < \frac{1}{6}$), the GEP gives energies to within 2% of the exact results even in the strong coupling limit. For the double-well potential ($m_B^2 < 0$) the GEP evolves, as $\hat{\lambda}$ increases, from a single-well shape, through a triple-well, to what is effectively a double-well shape. (Actually, the GEP always has a local minimum at the origin, but for large $\hat{\lambda}$ this becomes just a tiny, shallow dip at the top of the central barrier between the two deep wells.) In field theory one would describe this in terms of spontaneous symmetry breaking, with a first-order phase
transition from the symmetric vacuum at \( \phi_0 = 0 \) to a broken-symmetry vacuum at \( \phi_0 = \pm v \). The "critical \( \hat{\Lambda} \)" at which the non-trivial minimum becomes deeper than the one at the origin (\( \hat{\Lambda}_{\text{crit}} = 1.149 \)) would be viewed as the onset of the phase transition. In the QM case this language is, strictly speaking, not correct. Because of quantum-mechanical tunnelling through the barrier, the two would-be vacua at \( \phi_0 = \pm v \) can mix, and the true ground state is their symmetric combination. Thus the expectation value of \( \phi \) remains zero, and there is no true spontaneous symmetry breaking. However, once the barrier becomes sufficiently high, the tunnelling rate becomes so small that, for all practical purposes, there is symmetry breaking (viewing the system over some long, but finite, timescale). Thus, it is still convenient to talk about a "phase transition" from qualitatively different "single well" and "double well" regimes, even though this is a smooth, not a discontinuous, transition. [Above \( 1+1 \) dimensions the tunnelling becomes suppressed by a volume factor, and then one does have a true phase transition.] The GEP is very accurate both at small \( \hat{\Lambda} \) and at large \( \hat{\Lambda} \) (the latter being the "extreme double-well limit", where one has two well-separated harmonic wells). The GEP is less accurate in the transition region, where the error in the ground-state energy can be \( 10-15\% \).

In \( 1+1 \) dimensions, the integrals \( I_1 \) and \( I_0 \) become quadratically and logarithmically divergent, and a mass renormalization is necessary to obtain a finite effective potential. The renormalized GEP indicates a first-order phase transition from a single well to a double-well at \( \hat{\Lambda}_c = 2.553 \) [12].

In \( 2+1 \) dimensions, the integrals \( I_1 \) and \( I_0 \) diverge as \( \Lambda^2 \) and \( \Lambda \), respectively, where \( \Lambda \) is the ultraviolet cutoff. A mass renormalization is again required to renormalize the
GEP. As in 1+1 dimensions, the theory undergoes a SSB phase transition at $\lambda_c = 3.078$

In 3+1 dimensions, where the theory requires both mass and coupling-constant renormalizations, the GEP suggests the existence of two distinct theories: One of these is the "precarious" theory, which is characterized by an infinitesimal and negative bare coupling constant. This theory is stable, but only in the absence of an ultraviolet cutoff. The decay rate of the vacuum, otherwise finite, in fact vanishes as the cutoff is taken to infinity [16,12]. The other version of the theory, the so called "autonomous" version, is characterized by a positive infinitesimal bare coupling constant, and arises by also allowing an infinite renormalization of the expectation value of the field. The theory can in fact exhibit a SSB phase, and in its unbroken-symmetry phase the particles are massless [17,18].

1.4 Beyond the Gaussian Approximation

In this thesis, our objective is to improve upon the Gaussian approximation. We report results in two directions.

First, in the canonical Hamiltonian formalism, we study and employ the method of non-linear canonical transformations (NLCT) introduced by Polley and Ritschel [19,20]. The method allows one to perform variational calculations with non-Gaussian trial states, constructed by nonlinear unitary transformations acting on Gaussian states. We consider a non-trivial unitary transformation that leads to qualitative as well as quantitative improvement over the Gaussian approximation [21]. In particular we obtain a nontrivial analytical correction to the mass renormalization, with respect to the Gaussian case. For the $O(N)$-symmetric $\lambda(\phi^2)^2$ theory we derive explicit general formulas
for the expectation value of the Hamiltonian in a general NLCT state, and also derive a formula for the one-particle NLCT state energy.

Second, we report on the development of a manifestly covariant approach, based on the Euclidian path integral, to formulate a class of lower-bound approximations to $\Gamma_{1P1}$, the generating functional of one-particle-irreducible Green's functions [22,23]. In the Gaussian approximation the formalism allows us to compute the Gaussian effective action (GEA), as a natural variational bound to $\Gamma_{1P1}$. Consequently, we are able to obtain, non-trivially, the proper vertex functions at non-zero momenta, and at non-zero values of the classical field, from a fully variational calculation [24]. The formalism also allows us to consider improvement beyond the Gaussian approach, by applying nonlinear measure-preserving field transformations to the path integral. Effectively, we are able to evaluate the path integral with quartic field exponentials, instead of only quadratic field exponential (Gaussian) measures. For the $O(N)$-symmetric $\lambda(\phi^2)^2$ theory, we present an example that parallels the nonlinear canonical transformation of Ref. [21]. In 4 dimensions, we are able to renormalize the GEA, offering an interpretation of $\lambda_B\phi^4$ as a theory which undergoes SSB, but with noninteracting particles in the SSB phase [24]. As a second application of the GEA, we study the Higgs mechanism in scalar QED in the covariant gauge. In our variational framework, we are able to write down optimization equations for the GEA, and to optimize the gauge dependence of the effective potential, which selects the Landau gauge. We also obtain the renormalized effective potential.

The organization of the thesis is as follows. In Chapter 2, we review the Schrödinger canonical formalism and outline the NLCT method. In Chapter 3, we study the subject of nonlinear canonical transformations, and their application in quantum field theory.
In this Chapter we write down explicit formulas for the expectation value of the Hamiltonian, the one particle state energy, and survey several examples of nonlinear transformations. In Chapter 4, we consider in detail the $\pi^3$ transformation. In Chapter 5, the covariant formalism described in the previous paragraph is discussed. In Chapter 6, we derive the GEA $n$-point proper vertex functions, and renormalize the GEA. In Chapter 7, we discuss the scalar QED model. Finally in Chapter 8, we present our conclusions and outlook.
Chapter 2  The Schrödinger Canonical Formalism and the NLCT Method

In this chapter, we review the Schrödinger formalism, and the NLCT method. Our aim is to enrich the NLCT method, by considering a wider class of transformations than those considered in Refs. [20,25], increasing the power and appeal of the method.

2.1 The Schrödinger Canonical Formalism in Quantum Field Theory

The Schrödinger formalism [26,14], provides a simple framework whereby the quantization of a classical field theory parallels the standard quantization procedure in quantum mechanics, which leads to the Schrödinger equation for the wavefunction.

Consider a theory with a single scalar field $\phi$ with the classical Lagrangian density

$$\mathcal{L}(x) = \frac{1}{2} \partial_{\mu} \phi(x) \partial^{\mu} \phi(x) - V(\phi). \quad (2.1)$$

One can define the canonical momentum

$$\pi(x) = \frac{\partial \mathcal{L}(x)}{\partial \dot{\phi}(x)} \quad (= \dot{\phi}(x)). \quad (2.2)$$

Performing a Legendre transform, one can write the Hamiltonian density

$$\mathcal{H}(x) = \pi(x) \dot{\phi}(x) - \mathcal{L}(x)$$

$$= \frac{1}{2} \pi(x)^2 + \frac{1}{2} (\nabla \phi(x))^2 + V(\phi(x)). \quad (2.3)$$

To quantize the theory, the canonical fields $\phi$ and $\pi$ become operators in Hilbert space satisfying the equal-time commutation relations:

$$[ \phi(x), \phi(x') ] = 0, \quad (2.4)$$
\[ [\pi(x), \pi(x')] = 0, \quad (2.5) \]
\[ [\phi(x), \pi(x')] = i\hbar \delta(x - x'). \quad (2.6) \]

To proceed, as in quantum mechanics, one chooses a representation for the field operators. If \(|\Psi\rangle\) is a physical quantum state of the theory (i.e., a vector belonging to the Hilbert space in which the field operators are defined), then one can realize this state as a wavefunction (functional) in the \(\phi\) representation as

\[ \Psi[\phi] = \langle \phi | \Psi \rangle, \quad (2.7) \]

where the action of the field operator \(\phi(x)\) on the state \(|\Psi\rangle\) corresponds to ordinary multiplication:

\[ \phi(x)|\Psi\rangle \longrightarrow \phi(x)\Psi[\phi]. \quad (2.8) \]

In this representation, where \(\phi\) is diagonal, the action of the field momentum operator \(\pi(x)\) on the state \(|\Psi\rangle\) corresponds to a functional differentiation of the wavefunction:

\[ \pi(x)|\Psi\rangle \longrightarrow -i\hbar \frac{\delta}{\delta \phi(x)} \Psi[\phi]. \quad (2.9) \]

In addition, one defines the inner-product as a functional integral:

\[ \langle \Psi_1 | \Psi_2 \rangle = \int D\phi \ \Psi_1^\ast[\phi] \Psi_2[\phi]. \quad (2.10) \]

The energy eigenstates of the quantized theory satisfy the Schrödinger equation:

\[ H \Psi = E \Psi, \quad (2.11) \]

which written out in full reads (from now on we set \(\hbar = 1\)):

\[ \left\{ \int_x -\frac{1}{2} \frac{\delta^2}{\delta \phi(x) \delta \phi(x)} + \frac{1}{2} [\nabla \phi(x)]^2 + V(\phi(x)) \right\} \Psi[\phi] \]
= E \Psi[\phi]. \quad (2.12)

The standard time-independent Schrödinger equation of quantum mechanics can be
recovered as the zero dimensional version of the equation above. Of course, for the
multidimensional case, this functional differential equation is very hard to solve for a
general function \( V(\phi) \). However, this formulation provides a natural framework for
introducing variational methods in quantum field theory.

An upper bound to the ground state energy of the system, \( E_0 \), is given by the
Rayleigh-Ritz variational principle:

\[
\min_{\Psi} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_0. \quad (2.13)
\]

To be able to use this formula, we must be able to calculate expectation values of field
operators in the trial state \( |\Psi\rangle \). This is not feasible in general, since one can only readily
evaluate Gaussian functional integrals. We therefore begin by discussing a variational
calculation using a Gaussian wavefunctional. The NLCT method, discussed in the next
section, provides a means of performing variational calculations with a wider class of
trial wavefunctionals.

Technically, it is convenient to work in momentum space, employing the Fourier
transforms of the field \( \phi(x) \) and its conjugate \( \pi(x) \):

\[
\phi(p) = \int d^nx \ e^{-ip\cdot x} \phi(x),
\]

\[
\pi(p) = \int d^nx \ e^{ip\cdot x} \pi(x). \quad (2.14)
\]

The signs are such that

\[
[\phi(p), \pi(k)] = i \delta(p - k), \quad (2.15)
\]
and we employ the convention that \((2\pi)^\nu\) factors are to be associated with momentum space integrations, delta functions, and functional derivatives involving fields with momentum space arguments (\(\nu \equiv \text{no. of spatial dimensions}\)):

\[
\bar{\delta}(\mathbf{p}) \equiv (2\pi)^\nu \delta(\mathbf{p}),
\]  

\[
\int_\mathbf{p} \equiv \int \frac{d^\nu p}{(2\pi)^\nu},
\]  

\[
\pi(\mathbf{p}) = \frac{-i\bar{\delta}}{\delta \phi(\mathbf{p})} = -i(2\pi)^\nu \frac{\delta}{\delta \phi(\mathbf{p})}.
\]  

The Hamiltonian, \(H = \int d^\nu x \mathcal{H}\), for the \(\lambda_B \phi^4\) theory (with \(V = \frac{1}{2} m_B^2 \phi^2(x) + \lambda_B \phi^4(x)\)) can be written as:

\[
H = \int \left[ \frac{1}{2} \pi(\mathbf{p}) \pi(-\mathbf{p}) + \frac{1}{2}(\mathbf{p}^2 + m_B^2)\phi(\mathbf{p})\phi(-\mathbf{p}) 
\right.
\]

\[
+ \lambda_B \int_q \int_k \int_r \phi(\mathbf{p})\phi(\mathbf{q})\phi(\mathbf{k})\phi(\mathbf{r}) \bar{\delta}(\mathbf{p} + \mathbf{q} + \mathbf{k} + \mathbf{r}).
\]  

We shall be interested in evaluating expectation values of the form

\[
\langle \phi(\mathbf{p}_1) \cdots \phi(\mathbf{p}_n) \rangle \equiv \frac{\langle \Psi_0 | \phi(\mathbf{p}_1) \cdots \phi(\mathbf{p}_n) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}
\]  

where the Gaussian wavefunctional centered on \(\phi = 0\) (with \(p = |\mathbf{p}|\)) is:

\[
\Psi_0[\phi] = \sqrt{\mathcal{N}} \exp \left\{ -\frac{1}{2} \int \phi(\mathbf{p}) W(p) \phi(-\mathbf{p}) \right\}.
\]  

Thus:

\[
\langle \phi(\mathbf{p}_1) \cdots \phi(\mathbf{p}_n) \rangle = \mathcal{N} \int D\phi \phi(\mathbf{p}_1) \cdots \phi(\mathbf{p}_n) e^{-\int_p \phi(\mathbf{p}) W(p) \phi(-\mathbf{p})}.
\]  

where the normalization constant \(\mathcal{N}\) is chosen so that \(\langle \Psi_0 | \Psi_0 \rangle = 1\). To proceed one can use the trick of introducing a source term \(J(\mathbf{p}) \phi(-\mathbf{p})\) to write:

\[
\langle \phi(\mathbf{p}_1) \cdots \phi(\mathbf{p}_n) \rangle = \frac{\delta^n}{\delta J(\mathbf{p}_1) \cdots \delta J(\mathbf{p}_n)} \mathcal{N} \int D\phi e^{-\int_p \phi(\mathbf{p}) W(p) \phi(-\mathbf{p}) - \int_p J(\mathbf{p}) \phi(-\mathbf{p})} \bigg|_{J=0}.
\]  

(2.23)
The $\phi$ integration can be easily performed [52], yielding

$$
\langle \phi(p_1) \cdots \phi(p_n) \rangle = \frac{\delta^n}{\delta J(p_1) \cdots \delta J(p_n)} e^{\frac{1}{4} \int_p J(p) W^{-1}(p) J(-p)} \bigg|_{J=0}
$$

$$
\equiv \frac{\delta^n}{\delta J(p_1) \cdots \delta J(p_n)} G[J] \bigg|_{J=0}
$$

(2.24)

This formula provides a systematic way of performing expectation values. In addition, to evaluate expectation values of products of operators which involve $\phi$'s as well as $\pi$'s, one can first commute the $\pi$'s to the right, employing the commutation relations, and use the fact that

$$
\pi(p) |\Psi_0\rangle = -i \frac{\delta}{\delta \phi(p)} |\Psi_0\rangle
$$

$$
= i W(p) \phi(-p) |\Psi_0\rangle,
$$

(2.25)

eventually converting the original expression to a sum of expectation values of only $\phi$ operators. To illustrate how the present formalism works we can evaluate the expectation value of the Hamiltonian (2.19), with $\lambda_B = 0$. The expectation value of the $\pi^2$ term is:

$$
\langle \Psi_0 | \pi(p) \pi(-p) |\Psi_0\rangle = -\langle \Psi_0 | - W(p) \bar{\delta}(0) + W^2(p) \phi(p) \phi(-p) |\Psi\rangle
$$

$$
= W(p) \bar{\delta}(0) - W^2(p) \frac{\delta^2}{\delta J(p) \delta J(-p)} G[J] \bigg|_{J=0}
$$

$$
= W(p) \bar{\delta}(0) - W^2(p) \bar{\delta}(0) = \frac{1}{2} W(p) \bar{\delta}(0)
$$

(2.26)

In addition, we have already evaluated $\langle \Psi_0 | \phi(p) \phi(-p) |\Psi_0\rangle = \frac{1}{2} W^{-1}(p) \bar{\delta}(0)$. Hence:

$$
\langle \Psi_0 | H |\Psi_0\rangle = \frac{\bar{\delta}(0)}{4} \int_p W(p) + (p^2 + m_B^2) W^{-1}(p).
$$

(2.27)

By virtue of the Rayleigh-Ritz variational theorem, we can obtain an optimal upper bound on the vacuum energy by minimizing with respect to $W(p)$. Functional differen-
tiation with respect to $W(q)$ yields:

$$\frac{\delta}{\delta W(q)} \langle \Psi_0 | H | \Psi_0 \rangle = \frac{\delta(0)}{4} \left[ \int_p \delta(p - q) - (p^2 + m_B^2)W(p)\delta(p - q) \right]$$

$$= \frac{\delta(0)}{4} \left[ 1 - (q^2 + m_B^2)W^{-2}(q) \right]$$ (2.28)

Setting this expression equal to zero, gives $\tilde{W}^2(q) = q^2 + m_B^2$, and hence (2.27) results in $\tilde{\delta}(0)I_1(m_B) = (\tilde{\delta}(0)/2) \int_q \sqrt{q^2 + m_B^2}$ as an upper bound on the vacuum energy, which is the exact result. The quantity $\tilde{\delta}(0)$, is just the infinite space volume factor which we expect since we are dealing with the total vacuum energy, and not just the vacuum energy density.

Before we leave this section we establish the relation between the present formalism and the more familiar number representation in terms of annihilation and creation operators. The annihilation and creation operators can be defined as:

$$a_W(k) = W(k)\phi(-k) + \frac{\delta}{\delta \phi(k)},$$ (2.29)

$$a_W^\dagger(k) = W(k)\phi(k) - \frac{\delta}{\delta \phi(-k)}.$$ (2.30)

The operator $a_W(k)$ annihilates the state $|\Psi_0\rangle$. The commutation relation can be written as:

$$[a_W(k), a_W^\dagger(k')] = 2W(k)\delta(k - k').$$ (2.31)

### 2.2 The NLCT Method

As mentioned earlier, the effective potential can be derived in the Hamiltonian canonical formalism, by minimizing the expectation value of $\mathcal{H}$ over all possible states which have the expectation value of the operator $\phi(x)$ equal to the constant classical
field $\varphi_c$. The GEP is obtained by restricting these states to ones whose Schrödinger-representation wavefunctionals are of Gaussian form:

$$
\Psi_G[\phi] = \sqrt{N} \exp \left\{ -\frac{1}{2} \int_p \left[ \phi(p) - \phi_0 \bar{\phi}(p) \right] W(p) \left[ \phi(-p) - \phi_0 \bar{\phi}(p) \right] \right\}.
$$

(2.32)

Thus, the GEP can be viewed as a variational approximation to the effective potential:

$$
\overline{V}_G(\varphi_c) = \min_{\psi_G} \langle \psi_G | H | \psi_G \rangle,
$$

(2.33)

where, by a straightforward calculation, $\varphi_c \equiv \langle \psi_G | \phi | \psi_G \rangle = \phi_0$, and

$$
\langle \psi_G | H | \psi_G \rangle = J + \frac{1}{2} m^2_\hbar (I_0 + \phi_0^2) + \lambda_\hbar (\phi_0^4 + 6I_0\phi_0^2 + 3I_0^2),
$$

(2.34)

where

$$
I_N = \frac{1}{2} \int_k W(k)^{2N-1}, \quad J = \frac{1}{4} \int_k \left( W(k) + \frac{k^2}{W(k)} \right).
$$

(2.35)

Taking the functional derivative, it is easy to show that the optimum kernel function, $W(p)$, is \([14,31]\):

$$
W(p) = \sqrt{p^2 + \Omega^2}
$$

(2.36)

(so that $J$ reduces to $I_1(\Omega) - \frac{1}{2} \Omega^2 I_0(\Omega)$), with the mass parameter $\Omega$ given by \([27]\)

$$
\Omega^2 = m^2_\hbar + 12\lambda_\hbar [I_0(\Omega) + \phi_0^2].
$$

(2.37)

In most discussions of the GEP the form (2.36) is, quite naturally, assumed from the beginning. However, it is important in the present context to realize that it emerges from an optimization of a general kernel function $W(p)$. When we go on to consider non-Gaussian trial wavefunctionals, we will find that the optimum $W(p)$ is not necessarily of this form. (We will also find that the classical field $\varphi_c$ is no longer the same as the shift parameter $\phi_0$ in $\psi_G$.)
As mentioned earlier, in quantum field theory one can essentially evaluate only functional integrals with a Gaussian integral measure. This would indicate that one is limited to variational calculations with Gaussian trial wavefunctionals, as in the GEP. However the method of non-linear canonical transformations circumvents this apparent limitation. (Related methods have been employed in quantum mechanics [28], field theory [29], and in solid-state physics [30].) The NLCT method [19,20] consist of considering trial wavefunctionals of the form:

$$\Psi = U \Psi_G,$$  \hspace{1cm} (2.38)

where $\Psi_G$ is a normalized Gaussian wavefunctional, and $U$ is a unitary operator, $U = e^{-isB}$. The computation of the expectation value of $H$ in this state:

$$\langle \Psi | H | \Psi \rangle = \langle \Psi_G | U^\dagger H U | \Psi_G \rangle$$  \hspace{1cm} (2.39)

reduces to the calculation of the Gaussian expectation value of the "transformed Hamiltonian" $\bar{H} = U^\dagger H U$. Furthermore, $\bar{H}$ is easily constructed once one has computed the transforms of the field and its canonical conjugate:

$$\tilde{\phi}(\mathbf{p}) = U^\dagger \phi(\mathbf{p}) U, \quad \tilde{\pi}(\mathbf{p}) = U^\dagger \pi(\mathbf{p}) U,$$  \hspace{1cm} (2.40)

since the transform of $\phi^2$ is just $\tilde{\phi}^2$, etc. The unitary transformation of an operator $O$ is expressible as a multiple commutator series:

$$\tilde{O} = e^{isB} O e^{-isB} = \sum_{n=0}^{\infty} \frac{i^n}{n!} [B, O]_n,$$  \hspace{1cm} (2.41)

where $[B, O]_n = [B, [B, O]_{n-1}]$ and $[B, O]_0 = O$. With a suitable choice of the Hermitian operator $B$ one can arrange that the series truncates after the first non-trivial term. This then offers the prospect of a feasible calculation [32].
Possible operators $B$ can be constructed from products of $\phi$'s and $\pi$'s with various momentum arguments, $p_1, \ldots, p_n$. The momentum arguments must sum to zero to preserve translation invariance, but apart from this constraint we may include any function $f(p_1, \ldots, p_n)$. We call this the "correlator" and treat it as a "variational-parameter function" to be determined, ideally, by minimization of the energy. (The other variational-parameter function we have is the kernel in the Gaussian wavefunctional.) This procedure will lead to a variational approximation to the effective potential which can represent an improvement upon the GEP. Thanks to the Variational Principle we know that any lowering of the energy (for fixed bare parameters) represents an improvement.

The parameter $s$ serves as a convenient bookkeeping device, helping us to identify and organize the non-Gaussian terms. (Notice, however, that $s$ is really redundant, and could always be absorbed into the correlator, $f$.) With $s$ we may write:

$$\langle \Psi | H | \Psi \rangle = V_G + sV_1 + s^2V_2 + \cdots , \quad (2.42)$$

where $V_G$ is the Gaussian effective potential (GEP). If the linear term $V_1$ is non-zero we will certainly be able to lower the energy, and hence obtain an improvement over the GEP.

This approach was used in Refs. [20,25] with operators of the form:

$$B = \int_{p} \cdots \int_{q_1} f(p, q_1, \ldots, q_n) \pi(p) \phi(q_1) \cdots \phi(q_n) \delta(-p + q_1 + \cdots + q_n), \quad (2.43)$$

with a correlator of the form:

$$f(p, q_1, \ldots, q_n) = g(p, q_1, \ldots, q_n) h(p) k(q_1) \cdots k(q_n), \quad (2.44)$$
with

$$h(p) k(p) = 0. \quad (2.45)$$

This constraint ensures that the argument of the $\pi$ is never the same as the argument of any of the $\phi$'s, so that they will effectively commute. This then causes the multiple-commutator series, Eq. (2.41) to terminate after the first non-trivial term. However, it is hard to optimize the ansatz (one would need to introduce a Lagrange multiplier function to impose the constraint (2.45)), and so one is reduced to making rather ad-hoc guesses for the functions $h$, $k$, and $g$. References [20,25] used simple step-functions for $h$ and $k$ and took $g$ to be constant.

In this thesis we examine other transformations which do not require constraints on the correlator $f$ in order to be tractable. One can then hope to determine, at least approximately, the optimal form of the correlator $f$. We feel that this adds significantly to the power and elegance of the method. To find suitable operators $B$ we are guided by the following considerations: (i) As we shall see in the next chapter, operators $B$ which are only linear or quadratic in $\phi$'s and $\pi$'s do not produce non-Gaussian wavefunctionals, and so do not give any improvement upon the GEP. Thus, we must go to cubic operators, at least. (ii) Time reversal invariance, which implies that the wavefunctional is real, not complex, requires that $B$ should contain an odd number of $\pi$ factors. (iii) We want the multiple-commutator series (2.41) to truncate after the first non-trivial term [33]. For a theory with a single scalar field, these considerations leave us with a single possible cubic form for $B$; namely $B = \pi^3$. We shall study this transformation in detail in Chapter 4.

For an $O(N)$-symmetric theory with $N$ scalar fields one can distinguish "radial"
and “transverse” fields, where the radial direction in field space is that picked out by the classical field. This allows two other transformations which satisfy the above criteria; namely, \( B = \pi_R \phi^2 \) and \( B = \pi_R \pi \tau^2 \). The first of these is studied in Ref. [21], and we shall discuss the analog of this transformation in the covariant formulation in Section 5.3.
Chapter 3  Linear and Nonlinear Canonical Transformations

In this chapter we discuss the subject of canonical transformations in classical and quantum mechanics. Starting from the classical theory, we arrive at the generating functional for canonical transformations of the particular type relevant to this thesis. Next we show how the infinitesimal version of this formalism, together with the quantization rules, leads naturally to the corresponding quantum canonical transformations, and their generalization in quantum field theory. For $\lambda \phi^4$ we present explicit formulas for the expectation value of the Hamiltonian in NLCT states. Next, we derive a formula for the one particle state energy. Finally, we survey several examples of canonical transformations.

3.1 Canonical Transformations in Classical Mechanics

In this context, we present a brief summary since the subject is discussed in many textbooks [34]. Classical trajectories are known to satisfy the minimum action principle:

$$\delta S = \delta \int dt \, L,$$

$$= \delta \int dt \left[ p \dot{q} - H(p, q) \right] = 0,$$

which leads to the Hamilton equations of motion

$$\dot{q} = \frac{\partial H}{\partial p},$$

$$\dot{p} = -\frac{\partial H}{\partial q}.$$
where the variables $q$ and $p$ are the usual canonical variables. We can define a new set of variables $q'$ and $p'$ such that

$$
\delta \int dt [p \dot{q} - H(p, q)] = \delta \int dt [p' \dot{q}' - H'(p', q', t)] = 0,
$$

(3.5)

and

$$
\dot{q}' = \frac{\partial H'}{\partial p'},
$$

(3.6)

$$
p' = -\frac{\partial H'}{\partial q'},
$$

(3.7)

where the function $H'(p', q', t)$ is the new Hamiltonian. The new variables, which preserve the form of Hamilton equations, are said to be related to the old ones by a canonical transformation. It is often convenient to introduce generating functions from which canonical transformations can be explicitly constructed. Equation (3.5) implies the existence of a function $F = F(q, p, q', p', t)$ such that:

$$
p \dot{q} - H = p' \dot{q}' - H' + \frac{dF}{dt},
$$

(3.8)

and therefore:

$$
(p - \frac{\partial F}{\partial q}) dq + (-p' - \frac{\partial F}{\partial q'}) dq' - \frac{\partial F}{\partial p} dp - \frac{\partial F}{\partial p'} dp' + (H' - H - \frac{\partial F}{\partial t}) dt = 0.
$$

(3.9)

This equation is satisfied if the coefficients of the differentials are zero:

$$
\frac{\partial F}{\partial p} = 0, \qquad \frac{\partial F}{\partial p'} = 0,
$$

(3.10)

$$
p' = -\frac{\partial F}{\partial q'}, \qquad p = \frac{\partial F}{\partial q},
$$

(3.11)

and

$$
H' = H + \frac{\partial F}{\partial t}.
$$

(3.12)
To proceed, one can define four functionals of the form

\[ F_1 = F_1(q, p', t), \quad F_2 = F_2(q, p', t), \]
\[ F_3 = F_3(p, q', t), \quad F_4 = F_4(p, p', t), \]  
(3.13)

such that their Legendre transforms:

\[ F = F_1, \quad F = -q'p' + F_2(q, p', t), \]  
(3.15)
\[ F = qp + F_3(p, q', t), \]  
(3.16)
\[ F = qp - q'p' + F_4(p, p', t), \]  
(3.17)
\[ F = -q'p' + F_2(q, p', t), \]  
(3.18)

all satisfy eqs. (3.10-11). Of particular interest to us will be \( F_2 = F_2(q, p', t) \). From equations (3.10) and (3.11) it follows that

\[ q' = \frac{\partial F_2(q, p')}{\partial p'}, \]  
(3.19)
\[ p = \frac{\partial F_2(q, p')}{\partial q}. \]  
(3.20)

It is convenient to introduce a new function \( W = W(q, p') \) to write

\[ F_2 = qp' + W(q, p'), \]  
(3.21)

so that when \( W = 0 \), \( F_2 \) leads to the identity transformation: \( q' = q \), and \( p' = p \). The generalization of these formulas for systems with many degrees of freedom is straightforward: one regards the formulas above as valid for each degree of freedom. Thus, for instance, (3.19) and (3.20) would become:

\[ q_j' = \frac{\partial F_2(q, \{p'\})}{\partial p_j'}. \]  
(3.22)
\[ p_j = \frac{\partial F_2 \{ \{ q_i \}, \{ p'_i \} \}}{\partial q_j}. \quad (3.23) \]

A particular example of interest is:

\[ F_2 = p'_1 q_1 + p'_2 q_2 + s p'_1 q_2^2, \quad (3.24) \]

with \( W = s p'_1 q_2^2 \). Equations (3.22) and (3.23), readily lead to

\[ q'_1 = q_1 + s q_2^2, \quad (3.25) \]
\[ p'_1 = p_1, \quad (3.26) \]
\[ q'_2 = q_2, \quad (3.27) \]
\[ p'_2 = p_2 - 2 s q_2 p_1. \quad (3.28) \]

We should remark that to produce this canonical transformation, we could have started by specifying (3.25) and (3.26). We first find \( F_2 \) by integrating (3.22), with \( i = 1 \):

\[ F_2 = f(p'_2, q_1, q_2) + q_1 p'_1 + s q_2^2 p'_1, \quad (3.29) \]

where the function \( f \) is a "constant" of integration, independent of \( p'_1 \). By using equation (3.23) with \( i = 1 \), together with (3.26), we find:

\[ \frac{\partial f}{\partial q_1} = p_1 - p'_1 = 0, \quad (3.30) \]

which means that the function \( f = g(p'_2, q_2) \) is only a function of \( p'_2 \) and \( q_2 \). Using (3.22) with \( i = 2 \), we find

\[ q_2 = \frac{\partial g(p'_2, q_2)}{\partial p'_2}. \quad (3.31) \]

At this point, we are not committed to any particular choice of the function \( g \). Different choices of \( g \), would lead to different functions for \( q'_2 \) and \( p'_2 \). To reproduce (3.27) and
(3.28) we would need just the identity transformation: \( g = p_2 q_2 \). We could have also started with the transformations for the \( q \)'s, (3.25) and (3.27), and constructed the transformations for the \( p \)'s, (3.26) and (3.28). The moral here is that in general we do not need to guess, a-priori, the generator of a canonical transformation if we know how one or more of the variables transforms. We can derive from this information, both a generator and corresponding additional new variables that complete the canonical transformation, both choices being not unique.

### 3.2 Quantum Canonical Transformations

We shall now make a transition from the infinitesimal version of equation (3.21) to the concept of canonical transformations in quantum mechanics. We should remark that while canonical transformations in quantum mechanics are by no means new, the emphasis has been on transformations of expectation values, and not on the transformation properties of the operators themselves [30]. In the quantum mechanical setting, discussions of unitary transformations found in many textbooks do not make the connection with the classical theory of canonical transformations. One consequence of this omission is that while canonical transformations have played an instrumental role in the development of theoretical classical mechanics, more recently in nonlinear dynamics, their potential use and development in quantum mechanics are still not fully realized [30].

We shall now derive a parameterization of the new canonical variables in terms of a parameter \( s \), such that when \( s \) equals zero the new and old canonical variables are identical. One can express this parameterization in terms of Poisson commuta-
tors, amenable to the quantization rules, and consequently "derive" the corresponding quantum canonical transformations as unitary transformations of quantum mechanical operators. Consider thus the infinitesimal version of equation (3.21):

\[ F_2 = qp' + \epsilon G(q, p'), \]  

(3.32)

where epsilon is a small independent parameter. Equations (3.19) and (3.20), lead to

\[ q' = q + \epsilon \frac{\partial G}{\partial p'}, \]  

(3.33)

\[ p = p' + \epsilon \frac{\partial G}{\partial q}. \]  

(3.34)

The first of these equations, eq. (3.33), implies:

\[ q' = q + \delta q, \]  

(3.35)

\[ = q + \epsilon \frac{\partial G}{\partial p'}, \]  

(3.36)

\[ = q + \epsilon \frac{\partial G}{\partial p} + O(\epsilon^2). \]  

(3.37)

It follows then that \( \delta q = \epsilon \partial G/\partial p \), and similarly eq.(3.34) leads to \( \delta p = -\epsilon \partial G/\partial q \).

Hence:

\[ \delta q' = \frac{\partial q'}{\partial q} \delta q + \frac{\partial q'}{\partial p} \delta q, \]  

(3.38)

\[ = \epsilon \left[ \frac{\partial q'}{\partial q} \frac{\partial G}{\partial p} - \frac{\partial q'}{\partial q} \frac{\partial G}{\partial q} \right], \]  

(3.39)

\[ = \epsilon [q', G]_p, \]  

(3.40)

where

\[ [A, B]_p = \frac{\partial A}{\partial q} \frac{\partial B}{\partial p} - \frac{\partial A}{\partial p} \frac{\partial B}{\partial q}, \]  

(3.41)
is the Poisson bracket. Now, equation (3.40) can be written as a differential equation for \( q' = q'(s) \) where \( s \) is a parameter such that \( q'(0) = q \), i.e.:

\[
\frac{dq'}{ds} = [q', G]_P.
\]  

(3.42)

A formal solution for \( q'(s) \) is given in terms of its Taylor expansion:

\[
q'(s) = q'(0) + s \left. \frac{dq'}{ds} \right|_{s=0} + \left. \frac{1}{2} s^2 \frac{d^2 q'}{ds^2} \right|_{s=0} + \cdots,
\]  

(3.43)

but \( dq'/ds = [q', G] \), and \( d^2 q'/ds^2 = [[q', G], G] \), etc. Hence

\[
q'(s) = q + s[q', G]_{s=0} + \frac{1}{2} s^2 [[q', G], G]_{s=0} + \cdots.
\]  

(3.44)

The same result can be obtained for \( p' \):

\[
p'(s) = p + s[p', G]_{s=0} + \frac{1}{2} s^2 [[p', G], G]_{s=0} + \cdots.
\]  

(3.45)

In fact, it can be shown that for any analytic function \( u' = u'(q', p') \) one obtains:

\[
u'(p', q') = u(p, q) + s[u'(p', q'), G]_{s=0} + \frac{1}{2} s^2 [[u'(p', q'), G], G]_{s=0} + \cdots.
\]  

(3.46)

Applying the quantization rules, \( q \) and \( p \) become operators \( \hat{q}, \hat{p} \) in Hilbert space, and the Poisson bracket \( [A, B]_P \), becomes \(-i(\hat{A}\hat{B} - \hat{B}\hat{A})\). Hence, (3.44) and (3.45), using the Hausdorff formula, lead to

\[
\hat{q}' = e^{is\hat{G}} \hat{q} e^{-is\hat{G}},
\]  

(3.47)

\[
\hat{p}' = e^{is\hat{G}} \hat{p} e^{-is\hat{G}},
\]  

(3.48)

and also (3.46), dropping carets, leads to

\[
H'(q', p') = e^{is\hat{G}} H(q, p) e^{-is\hat{G}} = H(q', p').
\]  

(3.49)
The operator $G$ is just $dW/ds$ at $s = 0$ (since $W_{s=0} = 0$). The generator of the transformation, up to a possible operator-ordering ambiguity, can be constructed from knowledge of the transformation of one of the variables: Working in the classical formalism, as in the example of the previous subsection, one can first compute the functions $F_2$ and $W$ and from these obtain the operator $G$. To summarize, unitary transformations are the quantum analogue of classical canonical transformations. Hence, the transformed quantum operators are isospectral with respect to the original ones, and also preserve the Heisenberg commutation relations, e.g., $[q, p] = [q', p'] = i$.

3.3 Field Theory Formulas

As discussed in the previous chapter, NLCT states are constructed with unitary transformations acting on Gaussian states. In practice, for our purposes, we are interested in evaluating $\langle \Psi | H | \Psi \rangle = \langle \Psi_G | \tilde{H} | \Psi_G \rangle$, where $| \Psi \rangle = U | \Psi_G \rangle$, $\tilde{H} = U^\dagger H U$, and $U = \exp(-isB)$. Since $U$ is unitary, transformed products of $\phi$'s and $\pi$'s are equal to products of their transforms. Thus, the transformed Hamiltonian $\tilde{H}(\phi, \pi)$ can be written as $H(\tilde{\phi}, \tilde{\pi})$. The variables $\tilde{\phi}, \tilde{\pi}$ and $\phi, \pi$ are related by a canonical transformation. The new Hamiltonian is isospectral to the old one. To proceed, one evaluates the new canonical variables in terms of the old ones, and takes the Gaussian expectation value of $\tilde{H}$ in the original canonical variables. Although the procedure is mechanically simple, it has some fundamental significance. It is natural to think of $U$ as modifying the Gaussian state $\Psi_G$, thereby producing a more sophisticated trial state. Another point of view is that we are improving a variational bound on the lowest eigenvalue of an operator,
by estimating instead a bound for the lowest eigenvalue of an entire class of non-trivial operators isospectral to the original one. Having made this remark, we now turn to the details of the procedure, and derive specific formulas for the $O(N)$-symmetric $\lambda(\phi^2)^2$ theory.

Hereafter we shall abbreviate Gaussian expectation values $\langle \Psi_G | A | \Psi_G \rangle$ by $\langle A \rangle$. One first needs to compute the transformed $\phi$'s and $\pi$'s. Quite generally, these can be written in the forms:

$$\tilde{\phi}_R(p) = \phi_R(p) + \phi_0 \tilde{\delta}(p) + s\tilde{\phi}_R(p), \quad (3.50)$$
$$\tilde{\phi}_T(p) = \phi_T(p) + \tilde{s}\tilde{\phi}_T(p), \quad (3.51)$$
$$\tilde{\pi}_R(p) = \pi_R(p) + s\tilde{\pi}_R(p), \quad (3.52)$$
$$\tilde{\pi}_T(p) = \pi_T(p) + \tilde{s}\tilde{\pi}_T(p), \quad (3.53)$$

(where "R" and "T" refer to the radial and transverse fields, and where it should be understood that $\phi_T$, $\pi_T$, etc. are $O(N - 1)$ vectors). In general, the barred quantities will be power series in $s$, resulting from the multiple commutator series (2.41) of the previous chapter. For the specific transformation considered later the multiple commutator series will naturally truncate after, at most, one non-trivial term, and the barred quantities will then either vanish or be a single product of $\pi$'s. However, in this section we do not assume this simplification, and our formulas apply to a general, unitary transformation.

The un-transformed radial field $\phi_R$ has been redefined to include a shift $\phi_0 \tilde{\delta}(p)$, so that the Gaussian wavefunctional for the radial quantum field is now centered on $\phi_R = 0$ (i.e., so that $\langle \phi_R \rangle = 0$). However, in general, the additional terms generated by
the non-linear transformation will have non-zero Gaussian expectation value, so that the classical field, \( \varphi_c \), is not \( \phi_0 \). Instead we have:

\[
\varphi_c \, \delta(p) = \langle \Psi | \phi_R(p) | \Psi \rangle = \langle \tilde{\phi}_R(p) \rangle = \phi_0 \, \delta(p) + s \langle \tilde{\phi}_R(p) \rangle.
\] (3.54)

The \( \phi_0 \) parameter no longer has physical meaning and should be eliminated in favour of \( \varphi_c \). This can be done directly by substituting the last equation back into Eq. (3.50) above. The original shift \( \phi_0 \) was introduced as a free parameter, and by replacing it in favor of \( \varphi_c \), we are in effect choosing \( \phi_0 \) so that the expectation value of the field in our new NLCT state is any given value of \( \varphi_c \) we desire.

Having obtained the transformed \( \phi \)'s and \( \pi \)'s, it is straightforward to construct the transformed Hamiltonian, \( \tilde{H} \). The Gaussian expectation value of \( \tilde{H} \) can then be written in the following form (dropping an overall volume factor):

\[
\langle \tilde{H} \rangle = \langle \tilde{H}_R \rangle + \langle \tilde{H}_T \rangle + \lambda_B \left[ 2(N - 1)(I_0^R T_0^T + I_0^T \varphi_c^2) + s \beta_1^{RR} + s^2 \beta_2^{RT} + s^3 \beta_3^{RT} + s^4 \beta_4^{RT} \right],
\] (3.55)

where

\[
\langle \tilde{H}_R \rangle = J^R + s \, \kappa_1^R + s^2 \, \kappa_2^R + \frac{1}{2} m_2^2 (I_0^R + s \, \gamma_1^R + s^2 \, \gamma_2^R + \varphi_c^2)
\]

\[
+ \lambda_B \left[ 3(I_0^R)^2 + s \, \beta_1^R + s^2 \, \beta_2^R + s^3 \, \beta_3^R + s^4 \, \beta_4^R + 6 \varphi_c^2 (I_0^R + s^2 \, \gamma_2^R) + \varphi_c^4 \right],
\] (3.56)

and

\[
\langle \tilde{H}_T \rangle = (N - 1) J^T + s \, \kappa_1^T + s^2 \, \kappa_2^T + \frac{1}{2} m_2^2 \left[(N - 1) I_0^T + s \, \gamma_1^T + s^2 \, \gamma_2^T \right]
\]

\[
+ \lambda_B \left[ (N^2 - 1)(I_0^T)^2 + s \, \beta_1^T + s^2 \, \beta_2^T + s^3 \, \beta_3^T + s^4 \, \beta_4^T \right],
\] (3.57)

where \( J^R, J^T \), and the \( I_0 \) integrals are given in the previous chapter, and the \( \kappa, \beta, \) and
\( \gamma \) integrals are given below as follows:

\[
\kappa_i^R = \frac{1}{2} (\pi_R \pi_R + \pi_R \pi_R) + \frac{1}{2} \int_p p^2 \left\{ (\bar{\phi}_R(p) \phi_R(-p)) + (\phi_R(p) \bar{\phi}_R(-p)) \right\} \tag{3.58}
\]

\[
\kappa_2^R = \frac{1}{2} (\pi_R \pi_R) + \frac{1}{2} \int_p p^2 \left[ (\bar{\phi}_R(p) \phi_R(-p)) - (\bar{\phi}_R(p))(\bar{\phi}_R(-p)) \right], \tag{3.59}
\]

\[
\gamma_1^R = \langle \phi_R \bar{\phi}_R \rangle, \tag{3.60}
\]

\[
\gamma_2^R = \langle \bar{\phi}_R^2 \rangle - \langle \phi_R \rangle^2, \tag{3.61}
\]

\[
\beta_1^R = \langle \phi_R^3 \bar{\phi}_R \rangle + 4 \varphi_c \langle \phi_R^2 \bar{\phi}_R \rangle - 12 \varphi_c \langle \bar{\phi}_R \rangle \langle \phi_R^2 \rangle + 6 \varphi_c^2 \langle \phi_R \bar{\phi}_R \rangle, \tag{3.62}
\]

\[
\beta_2^R = \langle \phi_R^2 \bar{\phi}_R^2 \rangle - 4 \langle \bar{\phi}_R \rangle \langle \phi_R^2 \bar{\phi}_R \rangle + 6 \langle \bar{\phi}_R \rangle^2 \langle \phi_R^2 \rangle - 12 \varphi_c \langle \phi_R \bar{\phi}_R \rangle + 4 \varphi_c \langle \phi_R \bar{\phi}_R \rangle^2, \tag{3.63}
\]

\[
\beta_3^R = \langle \phi_R \bar{\phi}_R^3 \rangle - 4 \langle \bar{\phi}_R \rangle \langle \phi_R \bar{\phi}_R^2 \rangle + 6 \langle \bar{\phi}_R \rangle^2 \langle \phi_R \bar{\phi}_R \rangle + 4 \varphi_c \langle \phi_R \rangle^3 + 2 \langle \bar{\phi}_R \rangle^3 - 3 \langle \bar{\phi}_R \rangle^2 \langle \phi_R \rangle, \tag{3.64}
\]

\[
\beta_4^R = \langle \bar{\phi}_R^4 \rangle + 6 \langle \bar{\phi}_R \rangle^2 \langle \phi_R \rangle^2 - 4 \langle \bar{\phi}_R \rangle \langle \phi_R \rangle^3 - 3 \langle \phi_R \rangle^4. \tag{3.65}
\]

Where \( \langle \ldots \rangle \) means expectation value of all permutations of the enclosed operators, e.g.

\[
\langle \phi_R^3 \bar{\phi}_R \rangle = \langle \phi_R^3 \bar{\phi}_R + \phi_R \bar{\phi}_R \phi_R + \phi_R \bar{\phi}_R \phi_R + \phi_R \phi_R \bar{\phi}_R \rangle. \tag{3.66}
\]

For the transverse fields the expectation value \( \langle \phi_T \rangle \) will vanish, provided that the transformation preserves the \( O(N-1) \) symmetry among the transverse fields, and hence the formulas are simpler:

\[
\kappa_1^T = \frac{1}{2} \langle \pi_T \cdot \pi_T + \pi_T \cdot \pi_T \rangle + \frac{1}{2} \int_p p^2 \left\{ \langle \phi_T(p) \cdot \phi_T(-p) \rangle + \langle \phi_T(p) \cdot \phi_T(-p) \rangle \right\}, \tag{3.67}
\]

\[
\kappa_2^T = \frac{1}{2} \langle \pi_T \cdot \pi_T \rangle + \frac{1}{2} \int_p p^2 \langle \phi_T(p) \cdot \phi_T(-p) \rangle, \tag{3.68}
\]
\[ \gamma_1^T = \langle \phi_T \cdot \phi_T + \phi_T \cdot \phi_T \rangle, \] (3.69)
\[ \gamma_2^T = \langle \phi_T^2 \rangle, \] (3.70)

\[ \beta_1^T = \langle \phi_T^2 \phi_T \cdot \phi_T + \phi_T^2 \phi_T \cdot \phi_T + \phi_T \cdot \phi_T \phi_T^2 + \phi_T \cdot \phi_T \phi_T^2 \rangle, \] (3.71)

\[ \beta_2^T = \langle \phi_T^2 \phi_T \cdot \phi_T + \phi_T^2 \phi_T \cdot \phi_T + (\phi_T \cdot \phi_T)^2 + \phi_T \cdot \phi_T \phi_T \cdot \phi_T + \phi_T \cdot \phi_T \phi_T \cdot \phi_T \rangle, \] (3.72)

\[ \beta_3^T = \langle \phi_T \cdot \phi_T \phi_T \cdot \phi_T + \phi_T \cdot \phi_T \phi_T \cdot \phi_T + \phi_T \cdot \phi_T \phi_T \cdot \phi_T + \phi_T \cdot \phi_T \phi_T \cdot \phi_T \rangle, \] (3.73)

\[ \beta_4^T = \langle \phi_T^2 \phi_T \cdot \phi_T \rangle. \] (3.74)

The \( \beta^{RT} \) integrals are given by:

\[ \beta_1^{RT} = \langle \phi_R \phi_R \phi_T^2 + \phi_R \phi_R \phi_T^2 + \phi_R \phi_R \phi_T \cdot \phi_T + \phi_R \phi_R \phi_T \cdot \phi_T \rangle - 2\langle \phi_R \rangle \langle \phi_R \phi_T^2 \rangle - 2\phi_c \langle \phi_R \rangle \langle \phi_T^2 \rangle + c.c., \] (3.75)

\[ \beta_2^{RT} = \langle \phi_R^2 \phi_T^2 + \phi_R \phi_R \phi_T \cdot \phi_T + \phi_R \phi_R \phi_T \cdot \phi_T + \phi_R \phi_R \phi_T \cdot \phi_T + \phi_R \phi_R \phi_T \cdot \phi_T + \phi_R \phi_R \phi_T \cdot \phi_T \rangle - 2\langle \phi_R \rangle \langle \phi_R \phi_T^2 \rangle + \phi_c \langle \phi_T \cdot \phi_T + \phi_T \cdot \phi_T \rangle + c.c., \] (3.76)

\[ \beta_3^{RT} = \langle \phi_R \cdot \phi_T \cdot \phi_T + \phi_R \phi_T \cdot \phi_T + \phi_R \phi_T \cdot \phi_T + \phi_R \phi_T \cdot \phi_T + \phi_R \phi_T \cdot \phi_T \rangle - 2\langle \phi_R \rangle \langle \phi_R \phi_T^2 \rangle + \phi_c \langle \phi_T \cdot \phi_T \rangle + c.c., \] (3.77)

\[ \beta_4^{RT} = \langle \phi_R^2 \phi_T \cdot \phi_T \rangle - 2\langle \phi_R \rangle \langle \phi_R \phi_T \cdot \phi_T \rangle + \langle \phi_R \rangle \langle \phi_T \cdot \phi_T \rangle + c.c. \] (3.78)
Momentum arguments and integrations over them have been suppressed in the above formulas. Written out in full we would have, for example:

\[
\langle \phi \bar{\phi} \cdots \rangle = \int_{p_1} \int_{p_2} \cdots \int_{p_n} \langle \phi(p_1) \bar{\phi}(p_2) \phi(p_3) \cdots \rangle \delta(p_1 + p_2 + \cdots + p_n),
\]

\[
\langle \bar{\phi} \rangle^2 \langle \phi \phi \cdots \rangle = \int_{p_1} \int_{p_2} \cdots \int_{p_n} \langle \bar{\phi}(p_1) \rangle \langle \bar{\phi}(p_2) \rangle \langle \phi(p_3) \phi(p_4) \cdots \rangle \delta(p_1 + p_2 + \cdots + p_n).
\]

From inspection of the above formulas, obvious simplifications occur when the barred operators commute with the canonical fields (which unfortunately is not the case with the transformation of chapter 4). In addition, when the total number of fields in a single term is odd, the expectation value of this term vanishes. For \( N = 1 \), the are no transverse fields, and the relevant formulas are those with the radial "R" superscript only. The NLCT effective potential is obtained by optimizing \( \langle \bar{H} \rangle \) with respect to the variational-parameter functions \( W_R, W_T \), and the correlator(s) in the operator \( B \).

### 3.4 One-Particle-State Energy with NLCT States

In this section, we derive a formula for the one particle state energy, in the context of the NLCT formalism. We consider the \( N = 1 \) case here, but the resulting formula is easily generalized to the \( O(N) \) case. As in the Gaussian approximation, we define the one-particle creation operator as the Hermitian conjugate of the operator which annihilates the vacuum; in this case, the NLCT approximation to the vacuum: \( |\bar{\phi}\rangle = U|0\rangle \). In what follows, we shall use tildes to denote NLCT states. Consider the operator

\[
A(k) = U a(k) U^\dagger, \tag{3.79}
\]
where $a(k)$ is the standard annihilation operator (see eq. 2.29) of the Gaussian state, with kernel $W(k)$. The operator $A$ annihilates the NLCT vacuum, and therefore we define the NLCT one-particle state of momentum $k$ as:

$$|\tilde{k}\rangle = A^\dagger(k)|\tilde{0}\rangle$$  
$$= U a^\dagger(k)|0\rangle$$  
$$= U|k\rangle.$$  

(3.80)  
(3.81)  
(3.82)

The square of the normalization of these states is given by:

$$\langle \tilde{k} | \tilde{k} \rangle = \langle k | k \rangle$$  
$$= \langle 0 | [a(k), a^\dagger(k)] | 0 \rangle$$  
$$= 2W(k)\delta(0)\langle 0 | 0 \rangle.$$  

(3.83)  
(3.84)  
(3.85)

The one-particle energy, by definition, is:

$$E_1(k) = \frac{\langle \tilde{k} | \tilde{H} | \tilde{k} \rangle}{\langle k | k \rangle}$$  
$$= \frac{\langle k | \tilde{H} | k \rangle}{\langle k | k \rangle}.$$  

(3.86)  
(3.87)

But, since

$$|k\rangle = [a^\dagger(k) + a(-k)]|0\rangle$$  
$$= 2W(k)\phi(k)|0\rangle,$$

(3.88)  
(3.89)

using equations (3.85) and (3.87) we can write:

$$E_1(k) = \frac{2W(k)\langle 0 | \phi(-k)\tilde{H}\phi(k)|0\rangle}{\delta(0)}.$$  

(3.90)
We can simplify this formula further, and write it as the sum of two terms: the vacuum energy plus the energy contribution from the one-particle quantum. To this end, consider the quantity

\[
D(q) = \frac{\delta V_{\text{eff}}}{\delta W(q)} = \frac{\delta}{\delta W(q)} \left[ \frac{\langle 0 | \hat{H} | 0 \rangle}{\langle 0 | 0 \rangle} \right] = \left[ \frac{\delta \langle 0 | \hat{H} | 0 \rangle}{\delta W(q)} \langle 0 | 0 \rangle - \langle 0 | \hat{H} | 0 \rangle \frac{\delta \langle 0 | 0 \rangle}{\delta W(q)} \right] \langle 0 | 0 \rangle^{-2}. \tag{3.93}
\]

Since

\[
\frac{\delta \langle 0 | \hat{H} | 0 \rangle}{\delta W(q)} = \frac{\delta \langle 0 | \hat{H} | 0 \rangle}{\delta W(q)} + \langle 0 | \hat{H} \frac{\delta | 0 \rangle}{\delta W(q)} = -\frac{1}{2} \left[ \langle 0 | \phi(q) \phi(-q) \hat{H} | 0 \rangle + \langle 0 | \hat{H} \phi(q) \phi(-q) | 0 \rangle \right] \tag{3.94}
\]

\[
= -\langle 0 | \phi(-q) \hat{H} \phi(q) | 0 \rangle + \frac{1}{2} \langle 0 | \phi(-q) [\hat{H}, \phi(q)] + \text{h.c.} | 0 \rangle \tag{3.95}
\]

and

\[
\frac{\delta \langle 0 | 0 \rangle}{\delta W(q)} = -\langle 0 | \phi(-q) \phi(q) | 0 \rangle = -\frac{1}{2} W^{-1}(q) \delta \langle 0 | 0 \rangle, \tag{3.97}
\]

substituting back into (3.93), we obtain:

\[
D(q) = -\frac{\langle 0 | \phi(-q) \hat{H} \phi(q) | 0 \rangle}{\langle 0 | 0 \rangle} - \frac{1}{2} \frac{\langle 0 | \phi(-q) [\hat{H}, \phi(q)] + \text{h.c.} | 0 \rangle}{\langle 0 | 0 \rangle} + \frac{1}{2} W(q)^{-1} \frac{\langle 0 | \hat{H} | 0 \rangle}{\langle 0 | 0 \rangle}. \tag{3.98}
\]

The first term of the last equation is precisely, up to a factor, the right hand side of eq. (3.99). Hence, solving for this term, and substituting back into our formula for \( E_1 \) we can finally write:

\[
E_1(k) = V_{\text{eff}} + \frac{W(k)}{\delta \langle 0 | 0 \rangle} \frac{\langle 0 | \phi(-k) [\hat{H}, \phi(k)] + \text{h.c.} | 0 \rangle}{\langle 0 | 0 \rangle} - \frac{2W(k)}{\delta \langle 0 | 0 \rangle} D(k). \tag{3.99}
\]
The function $D(k)$, defined in (3.91), vanishes when the function $W$ is optimized. In addition, at the global minimum of the potential, $\varphi_c = \phi_v$, $V_{\text{eff}}$ becomes the vacuum energy, $E_0$. Thus, $E_1(k)$ is given by the formula:

$$E_1(k)|_{\varphi_c = \phi_v} = E_0 + \frac{W(k)}{\delta(0)} \left. \frac{\langle 0 | \phi(-k) [\tilde{H}, \phi(k)] + \text{h.c.} | 0 \rangle}{\langle 0 | 0 \rangle} \right|_{\varphi_c = \phi_v}. \quad (3.100)$$

As an example, we compute $E_1$ in the GEP approximation. The commutator in (3.100) becomes:

$$[\tilde{H}, \phi(k)] = [H, \phi(k)] \quad (3.101)$$

$$= \left[ -\frac{1}{2} \int_p \frac{\delta}{\delta \phi(p)} \frac{\delta}{\delta \phi(-p)} \phi(k) \right]. \quad (3.102)$$

After a little algebra, one obtains:

$$\langle 0 | \phi(-k) [\tilde{H}, \phi(k)] | 0 \rangle = -\langle 0 | \phi(-k) \frac{\delta}{\delta \phi(-k)} | 0 \rangle \quad (3.103)$$

$$= \frac{1}{2} \delta(0) \langle 0 | 0 \rangle. \quad (3.104)$$

Adding the Hermitian conjugate produces an additional factor of 2, and using equation (3.100) we obtain:

$$E_1(k) = E_0 + \tilde{W}(k), \quad (3.105)$$

where $\tilde{W}(k) = \sqrt{k^2 + \Omega^2}$, as expected. We should remark, however, that in general the momentum dependence of $E_1$, in our approximation, does not come from the function $W(q)$ alone, but also from the expectation value shown in (3.100). This means that although we have obtained a relativistically correct formula for the GEP case, this may not be the case for an arbitrary NLCT. This may be a reflection of the Hamiltonian formalism employed here which is not Lorentz covariant.
3.5 Examples of Canonical Transformations

In this section we survey several examples of canonical transformations. We first turn our attention to an example of a quadratic transformation, to show that, as mentioned in the previous Chapter, it does not improve upon the Gaussian approximation. Next, we discuss the simplest nonlinear transformation in the N=1 case, namely the "π^3" transformation. For the O(N) symmetric case we discuss the "π_π^2" transformation, studied in detail in references [21] and [35]. Finally, we explore a nontrivial transformation for the O(N) symmetric case which results in a non-terminating series for the transformed canonical fields, which can be nevertheless re-summed. Throughout this chapter we follow the notation and conventions introduced in the previous chapter.

Quadratic Transformations

Consider the following transformation in the context of quantum mechanics, specified by the operator:

\[ B = \frac{1}{2} s q^2. \]  

(3.106)

The transformed canonical coordinates become:

\[ \tilde{q} = q, \quad \tilde{p} = p + sq. \]  

(3.107)

In this case, transforming the Hamiltonian to the new canonical variables changes only the kinetic term proportional to p^2, since the transformation does not affect quantities dependent on q. Thus:

\[ \langle \tilde{p}^2 \rangle = \langle p^2 \rangle + s^2 \langle q^2 \rangle. \]  

(3.108)
Since the transformation changes the kinetic term by a positive definite term proportional to $s^2$, the transformation raises the energy with respect to the Gaussian ansatz. This is a general result: If the canonical transformation affects only the original conjugate momentum fields, $\pi(x)$, for theories with potentials which are only functions of $\phi(x)$, the transformation does not lead to an improvement over the Gaussian approximation. The reason is that the operator $B$, being only a function of $\phi$, results on a single term for $\bar{\pi}$ which is just the derivative $dB/d\phi$. Hence, only the Gaussian expectation value of the kinetic term is changed, by the addition of a single term which is proportional to $s^2$. This new term is always positive (with no linear terms in $s$) since otherwise, e.g., a quantity like $\Delta q \Delta p$, being lowered beyond its Gaussian lower limit, would result in a violation of the uncertainty principle.

Other choices for a quadratic $B$ operator lead to more interesting transformations, but with similar results. Consider for example:

$$B = \frac{1}{2} s(qp + pq),$$

(3.109)

which results in

$$\bar{q} = e^{-s} q, \quad \bar{p} = e^{s} p.$$  

(3.110)

Since $\langle q^2 \rangle = 1/(2\Omega)$ and $\langle p^2 \rangle = \Omega/2$, one can re-absorb the $s$ parameter in $\langle \bar{H} \rangle$ by redefining $\Omega$ to be $\Omega' = \exp(2s)\Omega$, which leads to the Gaussian approximation again.

The $\pi^3$ Transformation

In this subsection we introduce the $\pi^3$ transformation applied to the $N = 1$ theory. This is perhaps the simplest non-trivial example of the NLCT method. The unitary
operator $U = e^{-isB}$ is given by:

$$B = \frac{1}{3} \int_{p} \int_{q} \int_{r} f(p, q, r) \pi(p) \pi(q) \pi(r) \delta(p + q + r). \quad (3.111)$$

This transformation obviously leaves $\pi(p)$ unchanged. The commutator with $\phi(p)$ gives us directly $\overline{\phi}$ as:

$$\overline{\phi}(k) = \int_{q} \int_{r} f(k, q, r) \pi(q) \pi(r) \delta(k + q + r). \quad (3.112)$$

There are no higher terms in the multiple commutator series because this expression commutes with $B$. To check if the transformation is effective, in the sense of producing a linear term in $s$ in the expectation value of the Hamiltonian, we just need to compute $\beta_1$, using formula (3.62) of the previous chapter, resulting in:

$$\beta_1 = -2\varphi_c \int_{pq} f(p, q, r) \delta(p + q + r). \quad (3.113)$$

A study of the effects of this transformation in more detail is the subject of the next chapter.

**The $\pi_R\phi_T^2$ Transformation**

The following transformation, discussed in detail in refs. [21,35], illustrates how one can generate a nonlinear transformation mixing radial and transverse degrees of freedom in the $O(N)$-symmetric $\lambda\phi^4$ theory. The relevant $B$ operator in this case is

$$B = \int_{pq} f(p, q) \pi_R(p + q) \phi_T(p) \cdot \phi_T(q), \quad (3.114)$$

and the commutator series terminates after the first commutator, since $\pi_R$ commutes with $\phi_T$. The resulting barred fields are:

$$\overline{\phi}_R(k) = \int_{p} \int_{q} f(p, q) \phi_T(p) \cdot \phi_T(q) \delta(p + q - k),$$
\[
\bar{\pi}_\tau(k) = -2 \int_p f(p, k) \pi_N(p + k) \phi_\tau(p),
\]
\[
\bar{\pi}_N(k) = 0, \quad \bar{\phi}_\tau(k) = 0. \tag{3.115}
\]

The linear term in \(s\) is given by \(\beta^{RT}_1\), which can be written as
\[
\beta^{RT}_1 = 2\varphi_c(N - 1) \int_{pq} f(p, q) W^{-1}_T(p) W^{-1}_T(q). \tag{3.116}
\]

In Chapter 5, we shall derive in the context of the path integral formalism a transformation which produces parallel results to this transformation.

**Infinite Series Example**

To conclude this chapter, we present an example of a transformation that does not result in a terminating series; however, the resulting infinite series for the transverse barred fields can be resumed in matrix form. Consider the operator
\[
B = \frac{1}{2} \alpha^2 \int_{xyz} f_1(y - x, z - x) \pi_N(x) \pi_\tau(y) \pi_\tau(z)
+ \frac{1}{2} \beta^2 \int_{xyz} f_2(y - x, z - x) \pi_N(x) \phi_\tau(y) \phi_\tau(z). \tag{3.117}
\]

The computation of the transformed variables is straightforward and it leads to the following barred quantities:
\[
\bar{\phi}_N(r) = \frac{1}{2} \alpha^2 \int_{yz} f_1(y - r, z - r) \pi_\tau(y) \pi_\tau(z)
+ \frac{1}{2} \beta^2 \int_{yz} f_2(y - r, z - r) \phi_\tau(y) \phi_\tau(z), \tag{3.118}
\]

since \(B\) does not contain any \(\phi_N\)'s, \(\bar{\pi}_N(p) = 0\), and using
\[
\tilde{O} = \sum_{n=1}^{\infty} \frac{i^n}{n!} [B, O]_n, \tag{3.119}
\]
the barred transverse canonical fields become:

\[
\tilde{\phi}_T(r) = \alpha^2 \int_{xz} f_1(r - x, z - x) \, \pi_R(x) \, \pi_T(z) \\
- \frac{\alpha^2 \beta^2}{2} \int_{xz} f_1(r - x, z - x) \int_{x'z'} f_2(z - x', z' - x') \, \pi_R(x) \, \pi_R(x') \phi_T(z') \\
- \frac{\alpha^4 \beta^2}{6} \int_{xz} f_1 \int_{x'z'} f_2 \int_{x''z''} f_1 \, \pi_R(x) \, \pi_R(x') \, \pi_R(x'') \pi_T(z'') \\
+ \frac{\alpha^4 \beta^4}{24} \int_{xz} f_1 \int_{x'z'} f_2 \int_{x''z''} f_1 \int_{x'''z'''} f_2 \, \pi_R(x) \, \pi_R(x') \, \pi_R(x'') \, \pi_R(x'''') \phi_T(z''') + \cdots
\]

(3.120)

similarly,

\[
\bar{\pi}_T(r) = -\beta^2 \int_{xz} f_2(r - x, z - x) \, \pi_R(x) \, \pi_T(z) \\
- \frac{\alpha^2 \beta^2}{2} \int_{xz} f_2(r - x, z - x) \int_{x'z'} f_1(z - x', z' - x') \, \pi_R(x) \, \pi_R(x') \pi_T(z') \\
+ \frac{\alpha^4 \beta^4}{6} \int_{xz} f_2 \int_{x'z'} f_1 \int_{x''z''} f_2 \, \pi_R(x) \, \pi_R(x') \, \pi_R(x'') \phi_T(z'') \\
+ \frac{\alpha^4 \beta^4}{24} \int_{xz} f_2 \int_{x'z'} f_1 \int_{x''z''} f_2 \int_{x'''z'''}, f_1 \, \pi_R(x) \, \pi_R(x') \, \pi_R(x'') \, \pi_R(x''') \pi_T(z''') + \cdots
\]

(3.121)

Next, we can define the operator "matrices" (though with continuous, rather than discrete indices) \( \Pi_1 \) and \( \Pi_2 \) by their components in the continuum limit:

\[
\Pi_1(r, z) = \int_x f_1(r - x, z - x) \pi_R(x), \quad (3.122)
\]

\[
\Pi_2(r, z) = \int_x f_2(r - x, z - x) \pi_R(x), \quad (3.123)
\]

and regard \( \phi_T(z), \pi_T(z), \bar{\phi}_T(z), \) and \( \bar{\pi}_T(z) \) as "column vectors". With these definitions, we can conveniently employ "matrix" products. Since the components involved are now continuous variables, correspondingly all summations are replaced by integrals. Thus
for example, since $\Pi_1$ is a “matrix” and $\phi_T$ a “vector”, the product $\Pi_1\phi_T$ would be a “vector” with components:

$$\Pi_1\phi_T(r) = \int_{\mathbb{R}^3} \Pi_1(r, z)\phi_T(z),$$  \hspace{1cm} (3.124)

$$= \int_{\mathbb{R}^3} f_1(r-x, z-x)\pi_R(x)\phi_T(z).$$  \hspace{1cm} (3.125)

With these simplifications in the notation, the transverse barred fields can be rewritten as:

$$\bar{\phi}_T = \left[ \sum_{n=0}^{\infty} (-1)^n \frac{(\alpha \beta)^{2n}}{(2n)!} (\Pi_1 \Pi_2)^n \right] \phi_T - \phi_T$$  \hspace{1cm} (3.126)

$$+ \frac{\alpha}{\beta} \left[ \sum_{n=0}^{\infty} (-1)^n \frac{(\alpha \beta)^{2n+1}}{(2n+1)!} (\Pi_1 \Pi_2)^n \right] \pi_T,$$  \hspace{1cm} (3.127)

and

$$\bar{\pi}_T = \left[ \sum_{n=0}^{\infty} (-1)^n \frac{(\alpha \beta)^{2n}}{(2n)!} (\Pi_2 \Pi_1)^n \right] \pi_T - \pi_T$$  \hspace{1cm} (3.128)

$$- \frac{\beta}{\alpha} \left[ \sum_{n=0}^{\infty} (-1)^n \frac{(\alpha \beta)^{2n+1}}{(2n+1)!} (\Pi_2 \Pi_1)^n \right] \phi_T.$$  \hspace{1cm} (3.129)

Furthermore, defining:

$$\theta_{12}^2 = \Pi_1 \Pi_2, \quad \theta_{21}^2 = \Pi_2 \Pi_1,$$  \hspace{1cm} (3.130)

we can write

$$\bar{\phi}_T = \cos(\alpha \beta \theta_{12})\phi_T + \frac{\alpha}{\beta} \Pi_1 \theta_{21}^{-1} \sin(\alpha \beta \theta_{21})\pi_T - \phi_T,$$  \hspace{1cm} (3.131)

$$\bar{\pi}_T = \cos(\alpha \beta \theta_{21})\pi_T - \frac{\beta}{\alpha} \Pi_2 \theta_{12}^{-1} \sin(\alpha \beta \theta_{12})\phi_T - \pi_T.$$  \hspace{1cm} (3.132)

In quantum mechanics, the “matrices” $\Pi_{1,2}$ collapse to the canonical momentum $\pi_R$, hence the “matrices” $\theta_{ij}$ become just $\pi_R$ (with $f_i = 1$), and the formulas above become the scalar equations of Ref. [33].
Chapter 4    The $\pi^3$ Transformation and the Effective Potential

In this chapter we consider in more detail the $\pi^3$ transformation applied to the $N = 1 \lambda_B\phi^4$ theory. This is perhaps the simplest non-trivial example of the NLCT method in quantum field theory. For the $N = 1$ case there are no transverse fields, so the effective potential can be obtained just from Eq. (3.56) for $\langle \tilde{H}_R \rangle$, and we may drop the "R" superscript. Evaluating the Gaussian matrix elements involved (see Eqs. (3.58-3.65) in Chapter 3), we obtain:

\begin{equation}
\kappa_2 = \frac{1}{4} \int_p \int_q \int_r p^2 f^2(p,q,r)W(q)W(r) \delta(p + q + r),
\end{equation}

\begin{equation}
\gamma_2 = \frac{1}{2} \int_p \int_q \int_r f^2(p,q,r)W(q)W(r) \delta(p + q + r),
\end{equation}

\begin{equation}
\beta_1 = -2\varphi_c \alpha_1,
\end{equation}

\begin{equation}
\beta_2 = 6I_0 \gamma_2,
\end{equation}

\begin{equation}
\beta_3 = 4\varphi_c \alpha_3,
\end{equation}

\begin{equation}
\beta_4 = 3(\gamma_2^2 + \alpha_4),
\end{equation}

where the $\alpha$'s stand for

\begin{equation}
\alpha_1 = \int_p \int_q \int_r f(p,q,r)\delta(p + q + r),
\end{equation}

\begin{equation}
\alpha_3 = \int_{p_1} \int_{p_2} \int_{p_3} f(p_1 + p_2, -p_1, -p_2) f(p_1 + p_3, -p_1, -p_3) \times f(p_2 + p_3, -p_2, -p_3) W(p_1) W(p_2) W(p_3),
\end{equation}

\begin{equation}
\alpha_4 = \int_{p_1} \int_{p_2} \int_{p_3} \int_{p_4} f(p_1 + p_2, -p_1, -p_2) f(p_1 + p_3, -p_1, -p_3) \times f(p_2 + p_4, -p_2, -p_4) f(p_3 + p_4, -p_3, -p_4) W(p_1) W(p_2) W(p_3) W(p_4).
\end{equation}
Thus, $\langle \mathcal{H} \rangle$ can finally be written as:

\[
\langle \mathcal{H} \rangle = \langle \mathcal{H} \rangle_G + s^2 \kappa_2 + \frac{1}{2} m_B^2 s^2 \gamma_2 \\
+ \lambda_B \left[ -2 \varphi_c s \alpha_1 + 6s^2 (I_0 + \varphi_c^2) \gamma_2 + 4 \varphi_c s^3 \alpha_3 + 3s^4 (\gamma_2^2 + \alpha_4) \right],
\]

(4.10)

where the GEP part, $\langle \mathcal{H} \rangle_G$ is given by Eq. (2.34).

Note that in writing these expressions we have assumed that $f(p, q, r)$ is symmetric in its three arguments. There is obviously no loss of generality in so doing since only the symmetric part of $f$ contributes in Eq. (3.111). However, when attempting to optimize $f$, one should take care to explicitly symmetrize the above equations before taking a functional derivative with respect to $f$. (The point is that the functional derivative considers an arbitrary variation of $f$, and does not necessarily stay within the subspace of symmetric functions.) Also note that $f$ must be invariant under an overall rotation or inversion of our coordinate system. Therefore, in particular, $f(p, q, r) = f(-p, -q, -r)$.

Taking functional derivatives of Eq. (4.10) with respect to the kernel function $W(p)$ and the correlator $f(p, q, r)$ yields

\[
\frac{\delta \langle \mathcal{H} \rangle}{\delta W(k)} = \frac{\delta \langle \mathcal{H} \rangle_G}{\delta W(k)} + \frac{1}{2} \int_p \int_q s^2 f^2(p, q, k) \left[ (p^2 + \Omega^2) W(q) \right] \delta(p + q + k) \\
+ 12 \varphi_c s^3 \lambda_B \int_q \int_r \hat{f}(k, r) \hat{f}(q, -r) \hat{f}(k, r) W(q) W(r) + 6s^4 \lambda_B \gamma_2 \int_q \hat{f}^2(q, k) W(q) \\
+ 12s^4 \lambda_B \int_{p_1} \int_{p_2} \int_{p_3} \hat{f}(p_1, p_2) \hat{f}(p_1, p_3) \hat{f}(p_2, k) \hat{f}(p_3, k) W(p_1) W(p_2) W(p_3),
\]

(4.11)

\[
\frac{\delta \langle \mathcal{H} \rangle}{\delta f(p, q, r)} = \begin{cases} \\
-2s \lambda_B \varphi_c + \frac{s^2}{6} f(p, q, r) \left[ (p^2 + \Omega^2) W(q) W(r) \right] \\
+ (q^2 + \Omega^2) W(r) W(p) + (r^2 + \Omega^2) W(p) W(q) \right]
\end{cases} \\
+ 4 \lambda_B \varphi_c s^3 \int_t W(t) \left[ \hat{f}(-q, t) W(q) \hat{f}(r, t) W(r) \right]
\]
\[ + \hat{f}(-p, t)W(p)\hat{f}(r, t)W(r) + \hat{f}(-p, t)W(p)\hat{f}(q, t)W(q) \]
\[ + 2s^4\lambda_B\gamma_2 f(p, q, r)[W(q)W(r) + W(r)W(p) + W(p)W(q)] \]
\[ + 4s^4\lambda_B \int_{t_1}^{t_2} \int_{t_2}^{t_1} \hat{f}(t_1, t_2)W(t_1)W(t_2) \left[ \hat{f}(q, t_1)W(q)\hat{f}(r, t_2)W(r) + \hat{f}(p, t_1)W(p)\hat{f}(q, t_2)W(q) \right] \delta(p + q + r), \]
\[ (4.12) \]

where
\[ \hat{f}(q, r) = \int_p f(p, q, r)\delta(p + q + r), \]
\[ (4.13) \]

and
\[ \Omega^2 = m_B^2 + 12\lambda_B(I_0 + \varphi_c^2). \]
\[ (4.14) \]

Setting these derivatives to zero yields optimization equations that determine the optimal kernel and correlator. The product \( sf \) is proportional to \( \varphi_c \) near the origin, so we can solve the equations explicitly at \( \varphi_c = 0 \). In (4.11) only the Gaussian term survives, so that
\[ \overline{W}_0(p) = \sqrt{p^2 + \Omega_0^2}, \]
\[ (4.15) \]

where the zero subscript indicates a quantity evaluated at \( \varphi_c = 0 \). In (4.12) the first two terms dominate as \( \varphi_c \to 0 \), so that:
\[ s = 12\lambda_B\varphi_c, \]
\[ (4.16) \]

\[ \overline{f}_o(p, q, r) = \]
\[ \left[ (p^2 + \Omega_0^2)\overline{W}_0(q)\overline{W}_0(r) + (q^2 + \Omega_0^2)\overline{W}_0(r)\overline{W}_0(p) + (r^2 + \Omega_0^2)\overline{W}_0(p)\overline{W}_0(q) \right]^{-1} \]
\[ = \left[ \overline{W}_0(p)\overline{W}_0(q)\overline{W}_0(r) \left( \overline{W}_0(p) + \overline{W}_0(q) + \overline{W}_0(r) \right) \right]^{-1}. \]
\[ (4.17) \]
[Recall that only the product $sf$ is really meaningful: We have simply chosen to normalize $f$ in a convenient fashion, letting $s$ carry the other factors.] Stepping away from the origin, one could proceed to solve the equations iteratively, obtaining $\vec{f}$ and $\vec{W}$ as power series in $\varphi_c$.

The second derivative of the effective potential, $V = \min(\tilde{H})$, at the origin can be used to define a renormalized mass:

$$m_R^2 \equiv \frac{d^2V}{d\varphi_c^2} \bigg|_{\varphi_c=0}.$$

This is most conveniently obtained by first eliminating the redundant parameter $s$, setting it to be $12\lambda_B\varphi_c$, thereby making $\langle \tilde{H} \rangle$ manifestly an even function of $\varphi_c$. One can then obtain $m_R^2$ from a partial first derivative with respect to $\varphi_c^2$:

$$m_R^2 = 2 \left( \frac{dV}{d(\varphi_c^2)} \right)_{\varphi_c=0} = 2 \left( \frac{\partial(\tilde{H})}{\partial(\varphi_c^2)} \right)_{\varphi_c=0}.$$

Only the partial derivative is needed because the (functional) derivatives with respect to $f$ and $W$ vanish by virtue of the optimization equations. This gives

$$m_R^2 = \Omega_0^2 + 2(12\lambda_B)^2 \left( \kappa_2 + \frac{1}{2} \Omega_0^2 \gamma_2 - \frac{1}{6} \alpha_1 \right),$$

but from the $f$ equation (4.12), multiplied by $f(p,q,r)$ and integrated, we obtain the identity

$$\kappa_2 + \frac{1}{2} \Omega_0^2 \gamma_2 = \frac{1}{12} \alpha_1 \quad \text{(at $\varphi_c = 0$)}.$$

Therefore, the relationship between $m_R^2$ and $m_B^2$ is given by:

$$m_R^2 = \Omega_0^2 - 24\lambda_B^2 \alpha_1 |_{\varphi_c=0},$$

$$\Omega_0^2 = m_B^2 + 12\lambda_B I_0(\Omega_0).$$
In the Gaussian case we would have had $m^2 = \Omega_0^2$. The extra term involves the $\alpha_1$ integral of (4.7) evaluated with the $\varphi_c = 0$ forms of $f$ and $W$ above, which can be rewritten as:

$$ \alpha_1|_0 = \int_0^\infty dt \int d^\nu x \int_p \int_q \int_r e^{-i x \cdot (p+q+r)} \frac{1}{W_0(p)W_0(q)W_0(r)} e^{-[W_0(p)+W_0(q)+W_0(r)]t}, $$

where we have used the Fourier-transform form of $\delta(p + q + r)$. This integral reduces to:

$$ \alpha_1|_0 = 4 \int d^{\nu+1} x [G(x)]^3, $$

where

$$ G(x) = \int \frac{d^{\nu+1} p}{(2\pi)^{\nu+1}} \frac{e^{-ip\cdot x}}{p^\mu p_\mu + \Omega^2} $$

$$ = \int_p e^{-ix\cdot p} \frac{e^{-\omega|t|}}{2\omega} \quad (\text{with } \omega = W_0(p)), $$

is the (Euclidean) $x$-space propagator. In this form we recognize (4.22) as the same modification of the mass renormalization that one finds in second order in the post-Gaussian expansion [36]. In fact, $\alpha_1|_0$ corresponds to $\frac{2}{3} I^{(3)}$, the integral arising from the "barred circle" vacuum diagram. This is finite in $1+1$ dimensions, logarithmically divergent in $2+1$ dimensions (whereas the Gaussian term in the bare mass is linearly divergent), and quadratically divergent (like the Gaussian term) in $3+1$ dimensions. Unfortunately, this means that for dimensions greater than $1+1$, in cutoff regularization, the ansatz by virtue of (4.22) forces $\Omega_0$ to be infinite, or cutoff dependent. This seems to lead, by dimensional arguments, to an effective potential quartic in the classical field,
which indicates that although the theory undergoes SSB, the quantum, corrections to the renormalized effective potential become suppressed, albeit non-trivially. The handling of a cutoff dependent $\Omega$, however, is a very delicate matter and deserves further investigation before details can be reported.

4.1 The Second-Order Phase Transition in $1+1$ Dimensions

In $1+1$ dimensions, the GEP shows a first-order phase transition from the symmetric phase to the SSB phase [12]. At the origin, the GEP has always a local minimum, and hence the global minimum for the SSB phase develops away from the origin, indicating a first order phase transition. In contrast, the $\pi^3$ potential in $1+1$ dimensions shows a second-order phase transition, in accordance with a rigorous theorem [39]. In $1+1$ dimensions, $\alpha_1$ is finite ($\frac{2}{3}I^{(3)} = 2.344/(4\pi^2\Omega_0^2)$, [36]) and the renormalized mass at the origin vanishes when

$$\lambda_B = \lambda_c \equiv \left[ \frac{\Omega_0^2}{24\alpha_1|_{\phi_c=0}} \right]^{\frac{1}{2}} = 0.838\,\Omega_0^2,$$

(4.27)

Hence, $\lambda_c$ is the critical coupling constant for a second-order phase transition to SSB phase.

Polley and Ritschel [20], using a different NLCT ansatz, also obtained a second-order transition in their variational calculation (see also [37]).

An interesting feature of the present transformation, is that the renormalized mass at the origin is affected by three particle correlations through the integral $\alpha_1$. This integral corresponds, in perturbative language, to the “barred-circle” diagram which involves the interaction of three virtual particles of mass $\Omega$. In addition, as already mentioned, the same correction is also found in the delta-expansion to second order.
4.2 Numerical Results in 0 + 1 Dimensions

In quantum mechanics, with \( f = 1 \) and \( W(p) = \Omega \), \( \langle \tilde{H} \rangle \) becomes

\[
\langle \tilde{H} \rangle = \langle \mathcal{H} \rangle_G + \frac{1}{4} m_B^2 s^2 \Omega^2 + \lambda_B \left[ -2 \varphi_c s + 3 s^2 \Omega^2 \left( \frac{1}{2 \Omega} + \varphi_c^2 \right) + 4 \varphi_c s^3 \Omega^3 + \frac{15}{4} s^4 \Omega^4 \right]. \tag{4.28}
\]

The effective potential is obtained by minimizing this expression with respect to \( s \) and \( \Omega \), for each value of \( \varphi_c \). We have carried out this procedure numerically and in Figs. 4.1 and 4.2 we show the resulting potential, compared to the GEP, for two illustrative cases. As expected, the curves lie below the corresponding GEP curves. The two curves coincide at the origin because there the optimal value of \( s \) is zero. As \( |\varphi_c| \) increases, the optimal \( s \) becomes positive, and the optimal \( \Omega \) changes a little from its GEP value, resulting in a lowering of the effective potential.

As a quantitative measure of the degree of improvement we can examine the ground-state energy estimate, obtained from the value at the global minimum of the potential. This can be compared with the corresponding GEP estimate and with the exact result. For \( m_B^2 \) positive (the anharmonic oscillator case) the NLCT effective potential changes only insignificantly from the GEP and its minimum remains at the origin, yielding the same ground-state energy as the GEP. This value is within 2% of the exact result. For \( m_B^2 \) negative (the double-well case) there can be more significant changes in the shape and in the ground-state energy. A quantitative comparison is given in Table 1 (with "exact" results taken from the numerical calculations of [38]). As in Ref. [11] we use the dimensionless variable

\[
\zeta^2 = \frac{m_B^2}{(2 \lambda_B)^{1/3}}, \tag{4.29}
\]
and quote the energies, relative to the minimum of the classical potential, in units of $|m_{R}^{2}|$.

<table>
<thead>
<tr>
<th>$\zeta^{2}$</th>
<th>$E_{0}(\text{GEP})$</th>
<th>$E_{0}(\text{Exact})$</th>
<th>$%\text{Error(\text{GEP})}$</th>
<th>$%\text{Error (\pi^{3})}$</th>
</tr>
</thead>
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<td>0.705688</td>
<td>0.705686</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Table 1.

The NLCT calculation starts to yield lower ground-state energies than the GEP once $\zeta^{2} < -1.41278$, because then the global minimum moves away from the origin. For example, at $\zeta^{2} = -2$ (Fig. 4.1(a,b)), the GEP still has a single-well shape, but has developed lower minima away from the origin. For $\zeta^{2} = -4$ (Fig. 4.2(a,b)) both the GEP and have a double-well shape, but the latter has a lower minimum value. The GEP value is $13.79\%$ too large [40]; the NLCT calculation improves this, but only by an additional $3\%$. However, as we get into the “deep-double-well” region ($\zeta^{2} < -10$) the percentage error is reduced by an order of magnitude or more. Thus, the moral is that the NLCT method provides corrections to the GEP results in the same sense that a “second-order” calculation can be expected to improve a “first-order” one: That is, in the “transition region”, where the GEP itself is least accurate, the changes are large in absolute terms but small as a percentage of the actual error: In the “deep-double-well” region, where the GEP itself is quite accurate, the changes are small in absolute terms, but dramatically reduce the percentage error.

Next we discuss the changes in the shape of the potential. For this purpose, it is convenient to use the “renormalized parameters” $m_{R}, \tilde{\lambda}$ defined in Eqs. (1.23). As $\tilde{\lambda}$
Fig. 4.1. The effective potential for the NLCT $\pi^3$ (solid line) compared to the GEP (dashed line) and the classical potential (dotted line) in 0+1 dimensions, for $\zeta^2 = -2$. The GEP still has its minimum at the origin in this case. A closeup of the difference between the two effective potentials is shown in (b). (Units: $|m_B| = 1$)
Fig. 4.2. The effective potential for the NLCT $\pi^3$ (solid line) compared to the GEP (dashed line) and the classical potential (dotted line) in 0+1 dimensions, for $\zeta^2 = -4$. A closeup of the difference between the two effective potentials is shown in (b). (Units: $|m_B| = 1$)
increases the effective potential changes from a single-well to a double-well shape. This can be seen in Fig. 4.3, which compares the GEP and the $\pi^3$ effective potential. The GEP always has a local minimum at the origin, whereas for the $\pi^3$ potential the origin becomes a local maximum once $\hat{\lambda}$ exceeds $1/\sqrt{5}$, and a pair of shallow minima develop on either side of the origin. If we were in higher dimensions, this could be described as a "second-order phase transition". As $\hat{\lambda}$ is increased further, a second pair of minima appear, farther out from the origin, and these soon become deeper than the original pair of minima. This "first-order transition" happens at $\hat{\lambda} = 1.119$, very close to the "critical $\hat{\lambda}$" obtained in the GEP case.

This behavior can be seen in Fig. 4.4, which plots $\varphi_{\min}$, the value of $|\varphi_c|$ (in units of $m_R$) at which the global minimum of the effective potential occurs. (If we were in higher dimensions, $\varphi_{\min}$ would be the "order parameter" for a spontaneous-symmetry-breaking phase transition.) The general features of Fig. 4.4 — that the transition occurs "earlier" (at a lower $\hat{\lambda}$), and is "softer" (involves a smoother variation of $\lambda$) than the GEP would imply — seem to be true in 1+1 dimensions [20], and can also be expected to be true in higher dimensions as well.

To further appreciate how the $\pi^3$ potential works, it is useful to plot the wavefunction. The $\pi^3$ transformation changes the Gaussian wavefunction in momentum space by a $p$-dependent phase factor. Thus, the modulus of the wavefunction coincides with that of a Gaussian wavefunction of the same width in momentum space. However, these are not the same in coordinate space. The wavefunction in coordinate space can be obtained by performing a numerical Fourier transform from momentum space to coordinate space. In Fig. 4.5, the wave function at the vacuum is plotted together with
Fig. 4.3. The GEP (a) and the effective potential for the $\pi^3$ transformation (b) in 0+1 dimensions for $\lambda = 0.5, 1.0, 1.5, 2.0$ (from top to bottom).
Fig. 4.4. The value $\phi_{\text{min}}$ of $\varphi_c$ at the global minimum of the effective potential as a function of $\hat{\lambda}$ for the $\pi^3$ ansatz (dotted) and the GEP (solid). The ansatz shows a "second-order phase transition" at $\hat{\lambda} = 1/\sqrt{8}$ and a "first-order transition" at $\hat{\lambda} = 1.119$. 
the optimal Gaussian wave function for the same value of $\varphi_c$. As it can be seen, the effect of the transformation in the SSB region is to “distort” the Gaussian wavefunction so it becomes slightly asymmetric. This distortion correlates with the changes that one sees in the potential.
Fig. 4.5. The wavefunction that minimizes the energy for the NLCT $\pi^3$ (solid line) compared to the GEP wavefunction (dashed line) in 0+1 dimensions evaluated at the same classical field, for $\zeta^2 = -2$ (a), and $\zeta^2 = -4$ (b).
Chapter 5  Covariant Linear and Nonlinear Transformations

The Gaussian effective potential has been applied to many different field-theoretic models [41,42], and more recently, efforts have been made to go beyond the Gaussian approximation [19-21,36,43]. The results of the last Chapter are a part of these efforts.

There exist some disadvantages, however, pertaining to the conventional variational approach to relativistic field theories. One of these is that the Hamiltonian formalism, on which it is based, is not manifestly covariant. It is desirable from a practical point of view to perform calculations in a fully covariant formalism, which takes advantage of the Lorentz-symmetric treatment of space-time coordinates, especially since we are dealing with relativistic theories. Furthermore, as pointed out by Kovner and Rosenstein [44], certain popular renormalization prescriptions, such as the subtraction of UV-divergences at some space-like momentum, $p^2 = -M^2$, and the definition of the scattering amplitude at the symmetric point, $s = t = u = -M^2$, cannot be applied, since the effective potential contains information about the Green's functions only at zero momentum. Consequently, several attempts have been made to obtain the the effective action (EA), the generating functional of proper vertex functions (or one-particle irreducible Green's functions) with arbitrary momenta, from a variational calculation [44,45]. This work is based on the real-time formalism of Jackiw and Kerman [46]. In addition, beyond the benefits for renormalization, the calculation of nonperturbative proper vertex functions at nonzero momenta yields important information on multi-particle interactions.

In this Chapter, we describe a manifestly covariant variational scheme, based on the Euclidian path integral, which allows to calculate directly a nontrivial class of lower
bound approximations to $\Gamma_{PI}$, the generating functional of proper vertex functions [22,23]. For bosons this approximation can be derived from Feynman's variational principle [47] which, in turn, is an immediate consequence of Jensen's inequality for expectation values of convex functions; in particular, exponential functions:

$$\langle \exp(-S) \rangle \geq \exp(-\langle S \rangle).$$  \hspace{1cm} (5.1)

This inequality, as we shall see, leads to the Gaussian effective action (GEA) which generalizes the Gaussian effective potential (GEP). Furthermore, we propose a practical scheme to improve beyond the Gaussian approximation by considering nonlinear transformations of the fields under the path integral. For fermions, in general Jensen's inequality does not apply to functions of Grassmann numbers; however, a variational lower bound can be obtained if the procedure is equivalent to a variational calculation in the Hamiltonian formalism [48]. This is the case for variations of only the particle mass and it can be applied to the Gross-Neveu model [49]. One can also introduce nonlinear transformations in this context, by shifting left-handed spinors by a cubic function of the right-handed spinors [23].

The organization of the Chapter is as follows. In Section 5.1 we derive the approximation for the effective action based on the Feynman-Jensen inequality. In Section 5.2 we discuss the implementation of nonlinear field transformations as a means to improve upon the Gaussian approximation and present an application to the O(N)-symmetric $\lambda(\phi^2)^2$ model. Finally, in Section 5.3, we discuss the method in the context of Fermions.
5.1 The Effective Action

In the $O(N)$-symmetric $\phi^4$-model in $d$-dimensional Euclidian spacetime, the generating functional for Green’s functions is given by the functional integral

$$Z[j] = \int D\phi \ e^{-S\phi} \quad \text{where} \quad S\phi := S + \int_x j^a \phi^a$$

(5.2)

with $\int_x := \int d^d x$, and the action is

$$S = \frac{1}{2} \int_x \left( \partial_\mu \phi^a \partial^\mu \phi^a + m_B^2 \phi^a \phi^a \right) + \lambda_B \int_x (\phi^a \phi^a)^2,$$

(5.3)

where $a$ is summed over $1, \ldots, N$. In order to approximate $Z[j]$, we consider a class of transformations where the Jacobian is equal to unity:

$$\phi^a = f^a_\chi(\phi') \quad \text{such that} \quad D\phi = D\phi'$$

(5.4)

which depend on a number of free parameters $\chi$. These transformations, when applied to (5.3), amount to a class of actions $S\phi' = S' - j^a f^a_\chi(\phi')$ all generating the same $Z[j]$. Further, we introduce a test action

$$S_G = \frac{1}{2} \int_x \phi^a \phi'^b \left( G^{-1} \right)^{ab} \phi'^b,$$

(5.5)

with adjustable kernel $G$ to write $Z$ as

$$Z[j] = \int D\phi' \ e^{-S_G} e^{(S_G - S\phi')}.$$

(5.6)

Then, with the help of Feynman’s inequality (5.1), we obtain a variational lower bound

$$Z^A[j] = \max_{\chi,G} \left\{ \mathcal{N} \exp \left[ \mathcal{N}^{-1} \int D\phi' e^{-S_G} (S_G - S\phi') \right] \right\} \leq Z[j]$$

(5.7)

for the generating functional $Z[j]$. Since $S_G$ is quadratic in the fields, the normalization

$$\mathcal{N} = \int D\phi' \ e^{-S_G}$$

(5.8)
and the integral on the RHS of (5.7) can be calculated analytically. The kernel $G$ and the variational parameters $\chi$ in $f$ are to be optimized in (5.7).

The generating functional of connected Green’s functions as well as the free energy of the system coupled to the external source $j$ is given by $W = -\log(Z)$. As a consequence of the inequality for the $Z$'s,

$$W^A[j] := -\log(Z^A[j]) = \min_{\chi, G} \left\{ -\log(N) - N^{-1} \int D\phi^* e^{-S_\phi} (S_G - S_j) \right\} \quad (5.9)$$

forms an upper bound on $W$.

The more interesting object, however, is the EA of the model, often defined in textbooks [52] as the functional Legendre transform (denoted by $L$) of $W$,

$$\Gamma[\varphi_c] := LW[j] = \min_j \left\{ \int_x j\varphi_c - W[j] \right\}, \quad (5.10)$$

i.e., as the minimal “distance” between the straight line with slope $\varphi_c$ and $W$. Taking the Legendre transform of $W^A$, the resulting $\Gamma^A$ provides a lower bound on the EA. This follows from elementary properties of the Legendre transformation which will be discussed in more detail below.

One has to be careful, however, with the interpretation of $\Gamma$. As discussed by Dannenberg [50], the EA defined in (5.10) is not the generating functional of one-particle irreducible Green’s functions, $\Gamma_{1PI}$, but its concave envelope. $\Gamma$ is the double-Legendre transform of $\Gamma_{1PI}$, and differences occur if $\Gamma_{1PI}$ fails to be concave as in the case of spontaneously or dynamically broken symmetries. In the Hamiltonian formalism $\Gamma_{1PI}$ naturally emerges from calculations with trial wavefunctionals which are restricted to have a single peak localized around $\varphi_c[51]$.

We shall now derive a path-integral approximation $\Gamma^A_{1PI}$ which is (1) a lower bound
on $\Gamma_1^{PI}$ and (2) such that $W^A = L\Gamma_1^{A\pi}$. Consider the auxiliary functional

$$W^A[j; \chi, G] = -\log(N) - N^{-1} \int D\phi' e^{-S_G} (S_G - S - j^a f^a_{\chi}) \quad ,$$

(5.11)

i.e., the approximation for $W$ with the optimization in (5.9) not carried out. In addition let us define the function

$$\varphi^a(x) := N^{-1} \int D\phi' e^{-S_G} f^a_{\chi}(\phi'(x)) \quad ,$$

(5.12)

so that

$$W^A[j; \chi, G] = j^a \varphi^a - \log(N) - N^{-1} \int D\phi' e^{-S_G} (S_G - S) \quad .$$

(5.13)

Using Jensen's inequality for the functional-integral representation of $W$ and the correct [51] relation $W = L \Gamma_1^{PI}$ we obtain

$$W^A[j; \chi, G] \geq W[j] = j^a \varphi^a_c - \Gamma_1^{PI}[\varphi_c],$$

(5.14)

where $\varphi^a_c$ is the exact expectation value of the field, corresponding to a given source $j^a$. Since (5.14) is valid for arbitrary values of the parameters $\chi$ and $G$ in $W^A$ one can adjust them to satisfy the constraint $\varphi^a = \varphi^a_c$ where $\varphi^a$ is as in (5.12). Then the contributions $j^a \varphi^a_c$ appear on both sides of the inequality (5.14) and cancel exactly. By minimization in the constrained parameter space, one obtains

$$\Gamma_1^{A\pi}[\varphi_c] \equiv \max_{\chi, G} \left\{ \log(N) + N^{-1} \int D\phi' e^{-S_G} (S_G - S) \right\}_{\varphi_c \text{ fixed}} \leq \Gamma_1^{PI}[\varphi_c],$$

(5.15)

subject to the constraint

$$\varphi^a_c(x) = N^{-1} \int D\phi' e^{-S_G} f^a_{\chi}(\phi'(x)) \quad .$$

(5.16)
Hence $\Gamma^A_{1PI}[\varphi_c]$ is a lower bound on $\Gamma_{1PI}$. To show that $W^A = \mathcal{L}\Gamma^A_{1PI}$, consider the Legendre transform of $\Gamma^A_{1PI}$:

$$\mathcal{L}\Gamma^A_{1PI}[j] = \min_{\varphi_c} \left\{ \int_x j^a \varphi^a_c - \Gamma^A_{1PI}[\varphi_c] \right\}.$$  \hspace{1cm} (5.17)

Inserting (5.15) for $\Gamma^A_{1PI}$, the minimization with respect to $\varphi_c$ releases the constraint (5.16), and one obtains $W$ as in (5.9), with the unconstrained optimization of $\chi$ and $G$. Hence $W^A = \mathcal{L}\Gamma^A_{1PI}$.

The most elementary example for our scheme is the Gaussian effective action (for $N = 1$). In this case, the transformation consists in a shift of the field, $f_{\chi'} = \phi' + \chi$. Setting $\chi = \varphi_c$ satisfies (5.16). After performing the functional integrals, the lower bound on the EA is given by

$$\Gamma^{GEA}_{1PI}[\varphi_c] = \max_{\tilde{G}} \Gamma^{aux}[\varphi_c; G],$$ \hspace{1cm} (5.18)

where the auxiliary functional

$$\Gamma^{aux}[\varphi_c; G] = -\frac{1}{2} \int_p \left[ \log \tilde{G}^{-1} \right] (p, -p) - \frac{1}{2} \int_p \left( p^2 + m_B^2 \right) \left( \tilde{G}(p, -p) + \tilde{\varphi}_c(p)\tilde{\varphi}_c(-p) \right)$$ \hspace{1cm} (5.19)

$$- \lambda_B \int_{pqrs} \left( 3\tilde{G}(p, q)\tilde{G}(r, s) + 6\tilde{G}(p, q)\tilde{\varphi}_c(r)\tilde{\varphi}_c(s) + \tilde{\varphi}_c(p)\tilde{\varphi}_c(q)\tilde{\varphi}_c(r)\tilde{\varphi}_c(s) \right) \delta(p + q + r + s),$$ \hspace{1cm} (5.20)

where here and below we use Fourier amplitudes (as indicated by tildes) and the convenient notation $\int_p = 1/(2\pi)^d \int d^dp$, $\delta(p) = (2\pi)^d\delta(p)$.

The optimization equation for $\tilde{G}$, obtained by functional differentiation of $\Gamma^{GEA}_{1PI}[\varphi_c]$, can be written as

$$\tilde{G}(p, q) = (p^2 + m_B^2)\delta(p + q) + 12\lambda_B \int_{rs} \left[ \tilde{G}(r, s) + \tilde{\varphi}_c(r)\tilde{\varphi}_c(s) \right] \delta(p + q + r + s),$$ \hspace{1cm} (5.22)
which is equivalent to a truncated Dyson-Schwinger equation [44]. For a translationally invariant classical field $\varphi_c(x) = \varphi_c$ (and hence $\tilde{\varphi}_c(p) = \varphi_c \tilde{\delta}(p)$), $\tilde{G}$ is diagonal, and can be written as $\tilde{G}(p, q) = g(p) \delta(p + q)$, with

$$g(p) = \frac{1}{p^2 + \tilde{\Omega}^2}, \quad (5.23)$$

where $\tilde{\Omega}$ solves

$$\tilde{\Omega}^2 = m_B^2 + 12 \lambda_B \left( I_0 + \varphi_c^2 \right), \quad (5.24)$$

and $I_{-N} = \frac{4^N N!^2}{(2N)!} \int \frac{d^4 p}{(2\pi)^4} (p^2 + \tilde{\Omega}^2)^{-N-1}$ for $N \geq 0$. It can easily be shown that these integrals in $d = \nu + 1$ dimensions coincide with the $\nu$ dimensional integrals $I_n$ of Eq. (1.21). Hence, (5.24) reproduces the usual $\Omega$ equation for the GEP.

### 5.2 Implementing Nonlinear Field Transformations

In this section we discuss the implementation of nonlinear transformations $f^a_\chi$ leading to improvement beyond the GEA. As mentioned earlier, the idea is to perform a nonlinear transformation of the fields under the path integral, and then then compute $\Gamma^A_{IPJ}[\varphi_c]$, using a quadratic test action in the new fields, as in (5.5). To satisfy the condition $D\phi = D\phi'$, it is possible to construct several nonlinear transformations that lead to a Jacobian equal to unity. Consider for example

$$\tilde{\phi}^1(p) = f^1_\chi(\phi') = \tilde{\phi}^1(p) + \chi_0(p) + \sum_{a=2}^N \int_{qr} \chi_1(p, q, r) \tilde{\phi}^a(q) \tilde{\phi}^a(r) \delta(p - q - r) \quad (5.25)$$

$$\tilde{\phi}^a(p) = f^a_\chi(\phi') = \tilde{\phi}^a(p) \quad a = 2, \ldots, N \quad (5.26)$$

which is appropriate for studying spontaneous symmetry breaking $O(N) \to O(N - 1)$. The use of these nonlinear transformations in the path integral method is analogous to
the use of nonlinear canonical transformations in the Hamiltonian formalism. Accordingly, in the path integral formalism the original (untransformed) action is, effectively, evaluated with a test action $S_G$ which is not bilinear but quartic in the fields. The essential difference between the two formalisms is that whereas in the canonical formalism the transformations involve equal-time operators and their time derivatives, in the path integral formalism the transformations can be fully nonlocal. Thus for example, in quantum mechanics, these transformations can still correlate fields very far apart in Euclidian time.

It is possible to develop this approach further by considering nonlinear transformations in the context of the Hamiltonian path-integral formalism. With nonlinear canonical transformations, which automatically preserve the phase-space field measure $D\phi D\pi$, the method would proceed similarly whenever the exact path integral $Z$ can be transformed into Euclidian space.

We shall now turn to a concrete application of the present formalism, concerning the $O(N)$-symmetric $\phi^4$ theory. We discuss the transformation of equation (5.25), involving a mixing of the orthogonal degrees of freedom of the theory. A second example is presented in Refs. [22,23], for the $N = 1$ case in two dimensions, implementing a nonlinear transformation mixing even and odd degrees of freedom of the field. This transformation allowed to compute the critical coupling constant for the second order phase transition of the theory, which is not depicted by the Gaussian approximation, clearly establishing a practical application of the present method.
\section*{5.3 O(N)-Symmetric $\lambda(\phi^2)^2$}

In this section we consider an example of a nonlinear transformation that parallels the canonical nonlinear transformation of Section 3.3 [21,35]. Consider the action of equation (5.3). We separate the fields into a radial direction $\phi^R = \phi^1$, and a transverse $O(N-1)$ symmetric vector $\phi^T = (\phi^2, \ldots, \phi^N)$. The nonlinear transformation, we wish to consider is defined by:

\begin{equation}
\phi^R(x) = \phi^R(x) + s\phi^R_R(x) + \chi_0(x),
\end{equation}

\begin{equation}
\phi^T(x) = \phi^T_T(x),
\end{equation}

with

\begin{equation}
\phi^R_R(x) = \int_{y,z} f(y-x, z-x)\phi^T_T(y)\phi^T_T(z).
\end{equation}

The Jacobian of the transformation is unity, and hence the functional measure $D\phi = D\phi^t$. We introduce the quadratic test action:

\begin{equation}
S_G = \frac{1}{2} \int_{xy} \phi^R(x)G^{-1}_R(x,y)\phi^R(y) + \phi^T_T(x)G^{-1}_T(x,y)\phi^T_T(y)
\end{equation}

and set

\begin{equation}
\chi_0(x) = \varphi_c(x) - sN^{-1} \int D\phi^t e^{-S_G} \phi^R_R(x)
\end{equation}

in order to satisfy the constraint (5.16). The effective potential, for constant $\varphi_c$, becomes

\begin{equation}
V(\varphi_c) = V_G + \sigma^2 \chi_7 + \frac{1}{2}m^2_B \sigma^2 \chi_2 + \Lambda \{ 4\varphi_c s \chi_3 + \sigma^2[6I_0^R + 2(N - 1)I_0^T + 6\varphi_c^2] \chi_2 + 2s^2 \chi_5 + 4\varphi_c s^3 \chi_4 + 3s^4(\chi_6 + \chi_2^2) \},
\end{equation}

where $V_G$, the Gaussian result, is given by

\begin{equation}
V_G = \frac{1}{2} \int p \log \tilde{G}^{-1}_R(p) + \frac{N - 1}{2} \int p \log \tilde{G}^{-1}_T(p) + \frac{1}{2} \int p^2 (p^2 + m^2_B)(\tilde{G}_R(p) + (N - 1)\tilde{G}_T(p))
\end{equation}
\[ + \frac{1}{2} m_B^2 \varphi_c^2 + \lambda_B [3(I_0^R + \varphi_c^2)^2 - 2\varphi_c^4 + 2(N - 1)I_0^T (I_0^R + \varphi_c^2) + (N^2 - 1)I_0^T]^2 \] (5.33)

and

\[ I_0^R = \int_p \tilde{G}_R(p), \quad I_0^T = \int_p \tilde{G}_T(p). \] (5.34)

The \( \chi \) integrals are given by:

\[ \chi_2 = 2(N - 1) \int_{pq} \tilde{f}^2(p, q) \tilde{G}_T(p) \tilde{G}_T(q), \] (5.35)

\[ \chi_3 = 2(N - 1) \int_{pq} \tilde{f}(p, q) \tilde{G}_T(p) \tilde{G}_T(q), \] (5.36)

\[ \chi_4 = 8(N - 1) \int_{pqr} \tilde{f}(p, q) \tilde{f}(p, r) \tilde{f}(q, -r) \tilde{G}_T(p) \tilde{G}_T(q) \tilde{G}_T(r), \] (5.37)

\[ \chi_5 = 8(N - 1) \int_{pqr} \tilde{f}(p, q) \tilde{f}(p, r) \tilde{G}_T(p) \tilde{G}_T(q) \tilde{G}_T(r), \] (5.38)

\[ \chi_6 = 16(N - 1) \int_{pqrs} \tilde{f}(p, q) \tilde{f}(p, r) \tilde{f}(q, s) \tilde{f}(r, s) \times\tilde{G}_T(p) \tilde{G}_T(q) \tilde{G}_T(r) \tilde{G}_T(s), \] (5.39)

\[ \chi_7 = (N - 1) \int_{pq} (p + q)^2 \tilde{f}^2(p, q) \tilde{G}_T(p) \tilde{G}_T(q). \] (5.40)

As before, the tildes indicate Fourier amplitudes. The equations above resemble very much the canonical results [21], with the important distinction that all the integrals are over \( d \)-dimensional Euclidian momenta. In addition, the new \( \chi_7 \) integral is much simpler and leads to important simplifications as we shall see. Following a procedure analogous to reference [21], we optimize the function \( G_R, G_T \) and \( sf \). [As in the canonical formalism, only the product \( sf \) is really meaningful]. At the origin, the optimal functions \( \tilde{G}_R, \tilde{G}_T \) read:

\[ \tilde{G}_R(p) = \tilde{G}_T(p) = \frac{1}{p^2 + \Omega_0^2}, \] (5.41)

with

\[ \Omega_0^2 = m_B^2 + 4\lambda_B (N + 2) I_0^R [\tilde{G}_R]. \] (5.42)
The optimal correlator function \( \bar{f} \), fixing its normalization by setting \( s = -4\lambda_B \varphi_c \), satisfies an equation similar to equation (5.18) of reference [21]:

\[
\bar{f}(p, q) \left[ (p + q)^2 + \Omega_0^2 \right] = 1 - 8\lambda_B \int_r [\bar{f}(p, r) + \bar{f}(q, r)] \bar{G}_T(r),
\]

(5.43)

for which the solution is of the form:

\[
\bar{f}(p, q) = R(p, q)[1 + g(p) + g(q)].
\]

(5.44)

with the simpler covariant function

\[
R(p, q) = \frac{1}{(p + q)^2 + \Omega_0^2}.
\]

(5.45)

The function \( g(p) \) satisfies the linear integral equation

\[
g(p)[1 - h(p)] = h(p) - 8\lambda_B \int_r R(p, r)\bar{G}_T(r)g(r),
\]

(5.46)

with

\[
h(p) = -8\lambda \int_r R(p, r)\bar{G}_T(r) = -4\lambda I_{-1}(p).
\]

(5.47)

Thus for large \( p \), \( g(p) \) behaves as \( \lambda_B/p^{4-d} \), which can be neglected for space-time dimensions below \( d = 4 \), as far as the leading ultraviolet divergences are concerned. In addition, the renormalized mass at the origin reads:

\[
m_R^2 = \Omega_0^2 - 16^2\lambda_B \chi_3|_{\varphi_c=0}.
\]

(5.48)

If we take \( f \approx R \), then \( \chi_3 = \frac{N-1}{3}I^{(3)} \), as in [21]. The main advantage of the present formalism over the canonical approach is that the formulas for the \( \chi \) integrals, upon substitution of the optimal functions, simplify considerably. We should remark however, that although the present approach leads to the same mass renormalization of the
canonical approach, it may very well lead to a different renormalized effective potential. Although the structure of the \( s \) terms are similar in form to those found in the canonical formalism, the \( \chi \) integrals are different, and only \( \chi_3 \) can be shown to be the same, at the origin, in both formalisms.

5.4 Fermions

In theories that involve Fermions fields, quantum operators are antisymmetric with respect to the interchange of two fermion fields. Correspondingly, in the path integral formalism, the classical fermion fields that enter the classical action satisfy the anticommuting algebra of Grassman numbers. Unfortunately, Jensen's inequality does not hold for path integrals involving Grassman numbers, as we shall show in the following.

Grassman numbers, unlike ordinary real or complex numbers, obey the anticommuting algebra

\[
\eta_i \eta_j = -\eta_j \eta_i. \tag{5.49}
\]

As a consequence of (5.49), \( \eta_i \eta_i = 0 \), and hence a product of Grassman numbers is non-zero only if all the Grassman numbers are distinct. A function of \( n \) Grassman numbers is always of the form:

\[
F(\eta) = F^{(0)} + \sum_i F_i^{(1)} \eta_i + \sum_{ij} F_{ij}^{(2)} \eta_i \eta_j + \cdots + \sum_{ij \cdots n} F^{(n)} \eta_i \eta_j \cdots \eta_n, \tag{5.50}
\]

where the \( F^{(n)} \) are antisymmetric in all their indices. Grassman numbers also obey a different set of rules differentiation and integration, which are well explained in textbooks [2]. In particular, they satisfy the following Berezin integration rules:

\[
\int d\eta = 0, \tag{5.51}
\]
\[ \int d\eta \eta = 1, \quad (5.52) \]

If $\eta$ and $\eta'$ are $N$-dimensional column vectors, the Grassman integral

\[ \int d\eta d\eta' e^{\eta'^T M \eta} = \text{Det } M, \quad (5.53) \]

with

\[ d\eta d\eta' \equiv d\eta_1 d\eta'_1 \cdots d\eta_N d\eta'_N. \quad (5.54) \]

To show that Jensen's inequality does not hold for Grassman numbers, consider the integral (dropping the transpose $T$ superscript)

\[ I = \int d\eta d\eta' e^{\eta' + \lambda (\eta' \eta)} i. \quad (5.55) \]

The integrand can be expanded as follows:

\[ e^{\eta' + \lambda (\eta' \eta)} = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{m=0}^{\infty} \frac{\lambda^m}{m!} (\eta' \eta)^{n+m} \]

\[ = \sum_{m=0}^{[N/1]} \frac{\lambda^m}{m!(N-1m)!} (\eta' \eta)^N + \ldots, \quad (5.57) \]

where we have dropped in the last equation all the terms that will give zero when integrated. Hence, the integral can be readily evaluated to be

\[ I = N! \sum_{m=0}^{[N/1]} \frac{\lambda^m}{m!(N-1m)!}. \quad (5.58) \]

Suppose we introduce a test action $\alpha \eta' \eta$ and rewrite $I$ as:

\[ I = \int d\eta d\eta' e^{\alpha \eta' \eta + (1-\alpha) \eta' \eta + \lambda (\eta' \eta)} i. \quad (5.59) \]

then "Jensen's inequality" would suggest that the integral $I$ is bounded below by

\[ I_\alpha = N \exp \left[ N^{-1} \int d\eta d\eta' e^{-\alpha \eta' \eta (1-\alpha) \eta' \eta + \lambda (\eta' \eta)} i \right], \quad (5.60) \]
where the normalization factor

\[ N = \int d\eta d\eta' e^{\alpha^* \eta - \eta} = \alpha^N. \] (5.61)

After some algebra we obtain:

\[ I_\alpha = \alpha^N \exp \left[ N(\alpha^{-1} - 1) + \lambda \alpha^{-1} \frac{N!}{(N-l)!} \right]. \] (5.62)

For \( N = l = 2, I = 1 + 2\lambda, \) and with \( \alpha = 1, I_\alpha = \exp(2\lambda), \) which violates the inequality for \( \lambda > 0. \) It might appear that the inequality is reversed, i.e., that \( I_\alpha \geq I, \) but this is not the case since, for example, \( I_\alpha < I \) for \( \alpha = (1 + \sqrt{1 + 8\lambda})/2 \) with \( N = l = 2. \)

When the action corresponds to a Hamiltonian operator in Hilbert space a variational approximation can be formulated [48]. One example is the Gross-Neveu model [49], given by the (Euclidian) action

\[ S = \frac{i}{h} \int_p \bar{\psi}^a(p) \gamma_i \partial_i \psi^a(p) - h \int_{p,q,r,s} \bar{\psi}^a(p) \psi^a(q) \bar{\psi}^b(r) \psi^b(s) \delta(p + q + r + s). \] (5.63)

with \{\gamma_i, \gamma_j\} = -2\delta_{ij} (see [52]). Consider the “Gaussian” trial action:

\[ S_G = \frac{i}{h} \int_p \bar{\psi}^a(p) (\gamma_i \partial_i + \Omega) \psi^a(p), \] (5.64)

With the source term \( i \int_p \bar{\psi}^a(p) j(p) \psi^a(p) \) this leads to the Gaussian approximation for \( W \) [23]:

\[ W^A[j] = N_f \left\{ -2I_1(\Omega) + 2\Omega^2I_0(\Omega) + h_B(2N_f - 1)\Omega^2I_0^2(\Omega) + 2\Omega \int \frac{j(p)}{p^2 + \Omega^2} \right\}. \] (5.65)

This variational approximation corresponds to the approximation of Latorre and Soto [42] in the Hamiltonian canonical formalism, where by virtue of the Rayleigh-Ritz variational principle the mass \( \Omega \) can be optimized. Unfortunately, the approximation can
not be improved by nonlinear transformations as it can be done for the bosonic case by virtue of the Jensen inequality. Furthermore, for fermionic transformations which affect the time derivatives in the action, one can no longer invoke the Rayleigh-Ritz variational principle [48]. On the other hand, one can implement nonlinear fermionic transformations under the path integral, as pointed out by Polley [53], in order to incorporate nonperturbative correlations into a series expansion. As a concrete example, for the Gross-Neveu model, one can consider a nonlinear shift the left-handed spinor components by a polynomial in the right-handed components:

\[
\psi_L(p)' = \psi_L(p) + s \int_{qr} f(q,r,s) \delta(p - q - r - s) \psi_R(q)[\bar{\psi}_R(r)\psi_R(s)], \quad (5.66)
\]

\[
\bar{\psi}_L(p)' = \bar{\psi}_L(p) - \bar{s} \int_{qr} f(q,r,s) \delta(p - q - r - s) \bar{\psi}_R(q)[\bar{\psi}_R(r)\psi_R(s)], \quad (5.67)
\]

where the brackets indicate summations over the flavor and Dirac indices [23].
Chapter 6 Nonperturbative \(n\)-Point Functions from the Gaussian Effective Action and Renormalization of \(\lambda \phi^4\)

Spontaneous symmetry breaking (SSB) is the crucial ingredient of the Higgs mechanism in the Standard Model. Typically, the potential taken for the scalar sector is a suitable generalization of \(\lambda \phi^4\), which is renormalizable in perturbation theory. In the last decade, however, the existence of a nontrivial interacting \(\lambda \phi^4\) theory in 4 dimensions has been controversial [3]. In particular, the GEP suggests the existence of a nontrivial \(\lambda \phi^4\) theory with an infinitesimal positive bare coupling constant [55,17,18]. The theory was denominated “autonomous” because it is apparently quite separate from the perturbative version of the theory. In addition, it also evades other nonperturbative methods such as the conventional \(1/N\) expansion, and lattice calculations.

In the last chapter we described a fully covariant variational approach, based on Jensen’s inequality, to obtain a class of bounded approximations to \(\Gamma_{PI}\), the generating functional of one particle irreducible graphs [22]. The Gaussian effective action (GEA) emerged in this context as a natural lower-bound to \(\Gamma_{PI}\). Concerning the renormalization of the GEA, in the autonomous version of \(\lambda \phi^4\) the GEP is renormalized by an infinitesimal but positive bare coupling constant, \(\lambda_B \propto 1/I_{-1}\), and an infinite renormalization of the classical field, \(\varphi_c = \frac{1}{I_{-1}} \Phi_c\), where \(I_{-1}\) is proportional to the logarithm of the ultraviolet cutoff [17]. In contrast, when one tries to renormalize the GEA in this fashion, by rescaling the classical field \(\varphi_c(p)\), one finds that the kinetic term in the effective action spoils the renormalization. The situation can be clarified by considering a modification of the field renormalization, inspired by the background field method,
which amounts to regarding the ordinary classical field $\varphi_c(p)$ as a sum of a background constant field $B$ (zero-$k$ mode) plus a "shifted" field $Q_c(k)$ (with $Q_c(0) = 0$), each renormalized independently. In refs. [55] and [56], through a Renormalization Group (RG) analysis of the effective potential, the authors found that $\lambda \phi^4$ does undergo SSB, but that the shifted theory is a massive free field theory.

In the present chapter we apply this renormalization scheme to the GEA. We find, in accordance with refs. [55] and [56], that by taking the background field to be the constant translational invariant vacuum field configuration, and renormalizing this zero-$k$ mode of the field as in the GEP, we are left in the continuum limit with a renormalized GEA quadratic in the shifted field. Our findings suggest, however, after a functional expansion of the shifted theory involving the GEA $n$-point functions, that $\lambda \phi^4$ exhibits SSB but with *massless* free particles. The chapter is organized as follows. In Section 6.1, we describe a practical scheme to compute the GEA $n$-point functions, and present explicit expressions for the two-, three- and four-point functions, at nonzero momenta and evaluated at nonzero values of the classical field. Next, in Section 6.2 we perform our analysis of the shifted theory and present our conclusions.

### 6.1 The GEA $n$-Point Functions

To facilitate comparison with the situation in the GEP, we first derive expressions for the third and fourth derivative of the GEP with respect to $\varphi_c$. A few steps will seem unnecessary, but these will be useful for comparison with the derivation of $\Gamma_n$.

Consider the first $n$ derivatives of the GEP with respect to $\varphi_c$, at the optimal value
of $\Omega, \tilde{\Omega}$:

$$\frac{dV}{d\varphi_c} = m_B^2 \varphi_c + 12 \lambda_B I_0 \varphi_c + 4 \lambda_B \varphi_c^3, \quad (6.1)$$

$$\frac{d^2V}{d\varphi_c^2} = m_B^2 + 12 \lambda_B \left( I_0 + \varphi_c \frac{dI_0}{d\varphi_c} \right) + 12 \lambda_B \varphi_c^2, \quad (6.2)$$

and for $n \geq 3$:

$$\frac{d^nV}{d\varphi_c^n} = 24 \lambda_B (\delta_{n,3} \varphi_c + \delta_{n,4}) + 12 \lambda_B \left[ (n - 1) \frac{d^{n-2}I_0}{d\varphi_c^{n-2}} + \frac{d^{n-1}I_0}{d\varphi_c^{n-1}} \right]. \quad (6.3)$$

The last equation can be rewritten by noting that for $n \geq 1$:

$$\frac{d^n\tilde{\Omega}}{d\varphi_c^n} = 12 \lambda_B \frac{d^nI_0}{d\varphi_c^n} + 24 \lambda_B (\delta_{n,1} \varphi_c + \delta_{n,2}). \quad (6.4)$$

Hence, for $n \geq 3$:

$$\frac{d^nV}{d\varphi_c^n} = -48 \lambda_B (\delta_{n,3} \varphi_c + \delta_{n,4}) + (n - 1)\theta_{n-2} + \theta_{n-1} \varphi_c, \quad (6.5)$$

with

$$\theta_n \equiv \frac{d^n\tilde{\Omega}}{d\varphi_c^n}. \quad (6.6)$$

To make further progress, the $\theta$'s have to be given in terms of the familiar $I_N$ integrals.

To this end, consider the equation for $\theta_1$:

$$\begin{align*}
\theta_1 &= 24 \lambda_B \varphi_c + 12 \lambda_B \frac{dI_0}{d\varphi_c} \\
&= 24 \lambda_B \varphi_c - 6 \lambda_B I_{-1} \theta_1 \\
&= k_1 - 6 \lambda_B I_{-1} \theta_1,
\end{align*} \quad (6.7)$$

where we have introduced the quantity $k_1$ which is independent of $\theta_1$, thus allowing us to solve for $\theta_1$. Differentiating once more, one obtains:

$$\theta_2 = k_2 - 6 \lambda_B I_{-1} \theta_2, \quad (6.10)$$
with

\[ k_2 = 24 \lambda_B + 12 \lambda_B \frac{d^2 I_0}{d \varphi_c d \Omega^2} \theta_1. \] (6.11)

\( k_2 \) now depends on \( \theta_1 \), but not on \( \theta_2 \). In this fashion we can obtain \( \theta_m \) recursively, given \( k_m \), in terms of \( \theta_1, \ldots, \theta_{m-1} \). After some algebra one obtains:

\[ \theta_1 = 24 \lambda_B (1 + 6 \lambda_B I_{-1})^{-1}, \] (6.12)

\[ \theta_2 = 12 \lambda_B (1 + 6 \lambda_B I_{-1})^{-1} \left( 2 + \frac{3}{4} \theta_1^2 I_{-2} \right) \]
\[ = 24 \frac{\lambda_B}{1 + 6 \lambda_B I_{-1}} + 5184 \frac{\lambda_B^3 \varphi_c^2 I_{-2}}{(1 + 6 \lambda_B I_{-1})^3}, \] (6.13)

\[ \theta_3 = 12 \lambda_B (1 + 6 \lambda_B I_{-1})^{-1} \left( \frac{9}{4} \theta_1 \theta_2 I_{-2} - \frac{15}{8} \theta_1 I_{-3} \right) \]
\[ = 15552 \frac{\lambda_B^3 \varphi_c I_{-2}}{(1 + 6 \lambda_B I_{-1})^4} - 311040 \frac{\lambda_B^3 \varphi_c^3 I_{-3}}{(1 + 6 \lambda_B I_{-1})^4} \]
\[ + 3359232 \frac{\lambda_B^5 \varphi_c^3 I_{-2}^2}{(1 + 6 \lambda_B I_{-1})^5}. \] (6.14)

Finally, using (6.5), the third and fourth derivative are given by:

\[ \frac{d^3 V}{d \varphi_c^3} = -48 \lambda_B \varphi_c + 72 \frac{\lambda_B \varphi_c}{1 + 6 \lambda_B I_{-1}} + 5184 \frac{\lambda_B^3 \varphi_c^2 I_{-2}}{(1 + 6 \lambda_B I_{-1})^3} \] (6.15)

and

\[ \frac{d^4 V}{d \varphi_c^4} = -48 \lambda_B + 72 \frac{\lambda_B}{1 + 6 \lambda_B I_{-1}} + 31104 \frac{\lambda_B^3 \varphi_c^2 I_{-2}}{(1 + 6 \lambda_B I_{-1})^3} \]
\[ - 311040 \frac{\lambda_B \varphi_c I_{-3}}{(1 + 6 \lambda_B I_{-1})^4} + 3359232 \frac{\lambda_B^5 \varphi_c^3 I_{-2}^2}{(1 + 6 \lambda_B I_{-1})^5}. \] (6.16)

As a check of our procedure, we can directly differentiate the expression for the second derivative given in GEP II (eq. 3.15). First, we rearrange it a bit:

\[ \frac{d^2 V}{d \varphi_c^2} = m_B^2 + 12 \lambda_B (I_0 + \varphi_c^2) - \frac{(12 \lambda_B \varphi_c)^2 I_{-1}}{1 + 6 \lambda_B I_{-1}} \] (6.17)
\[ = m_B^2 + 12 \lambda_B I_0 - 12 \lambda_B \varphi_c^2 + \frac{24 \lambda_B \varphi_c^2}{1 + 6 \lambda_B I_{-1}} \] (6.18)
Thus:

\[
\frac{d^3V}{d\varphi_c^3} = 12\lambda_B \frac{d I_0}{d\varphi_c} - 24\lambda_B \varphi_c + 48 \frac{\lambda_B \varphi_c}{1 + 6\lambda_B I_{-1}} + 5184 \frac{\lambda_B^3 \varphi_c^2 I_{-2}}{(1 + 6\lambda_B I_{-1})^3} \\
= (\frac{d \Omega^2}{d\varphi_c} - 24\lambda_B \varphi_c) - 24\lambda_B \varphi_c + 48 \frac{\lambda_B \varphi_c}{1 + 6\lambda_B I_{-1}} + 5184 \frac{\lambda_B^3 \varphi_c^2 I_{-2}}{(1 + 6\lambda_B I_{-1})^3} \\
= -48\lambda_B \varphi_c + 72 \frac{\lambda_B \varphi_c}{1 + 6\lambda_B I_{-1}} + 5184 \frac{\lambda_B^3 \varphi_c^2 I_{-2}}{(1 + 6\lambda_B I_{-1})^3}. 
\]

(6.19)

In addition, direct differentiation of \(d^3V/d\varphi_c^3\) reproduces \(d^4V/d\varphi_c^4\) as it was previously obtained.

We now turn our attention to the GEA. The proper vertices for \(\lambda \phi^4\) obtained from the GEA, are the same as those obtained in the Covariant Gaussian Approximation of Kovner and Rosenstein [44]. In references [22] and [44], explicit expressions were given for the two-point function, and four-point function. The latter was given evaluated at \(\varphi_c = 0\), corresponding to a zero classical field. However, in the autonomous version of \(\lambda \phi^4\), the fourth derivative of the effective potential is singular at the origin, due to the \(\varphi_c^4 \ln \varphi_c\) term in the GEP, and hence the four-point function must be evaluated away from the origin.

A difficulty in computing \(n\)-point functions in a variational approximation is that the variational parameters in general are functionals of the classical field. This means, that since \(n\)-point functions are total functional derivatives of the action, one must take functional derivatives of the variational parameters with respect to the classical field. In the GEP formalism, for a constant classical field configuration, the Gaussian kernel \(G(p, q)\) becomes upon optimization a diagonal function in momentum space:

\[
G(p, q) = \frac{(2\pi)^d \delta^d(p + q)}{p^2 + \Omega^2}, 
\]

(6.20)
where the parameter $\tilde{\Omega}$ is an ordinary function of the constant classical field $\varphi_c$. However, in computing $n$-point functions, even though they will be evaluated at constant $\varphi_c$, one must allow for arbitrary variations of the classical field when taking the functional derivatives. This in turn means that in the Gaussian approximation one must employ the optimal Gaussian kernel for an arbitrary—non-translationally invariant—field configuration, which in general is a non-diagonal function. In this case the optimal kernel is given implicitly by an integral equation, and the calculation can become very cumbersome. The $n$-point functions are defined by the functional Taylor expansion of $\Gamma_{1P1}$:

$$\Gamma[\tilde{\varphi}_c] = \sum_n \frac{1}{n!} \int_{p_1 \cdots p_n} \Gamma_n(p_1, \ldots, p_n)[\tilde{\varphi}_c(p_1) - \varphi_c \delta(p_1)] \cdots \tilde{\varphi}_c(p_n) - \varphi_c \delta(p_n)], \quad (6.21)$$

where here and below we use Fourier amplitudes (as indicated by tildes) and the convenient notation of Chapter 5: $\int_p = 1/(2\pi)^d \int d^dp$, $\delta(p) = (2\pi)^d \delta(p)$, $\delta/\delta \varphi_c(p) = (2\pi)^d \delta/\delta \tilde{\varphi}_c(p)$. Hence:

$$\Gamma_n(p_1, \ldots, p_n) = \left. \frac{\delta^n \Gamma[\tilde{\varphi}_c]}{\delta \tilde{\varphi}_c(p_1) \cdots \delta \tilde{\varphi}_c(p_n)} \right|_{\tilde{\varphi}_c(p) = \varphi_c \delta(p)}. \quad (6.22)$$

As shown in ref. [22], a lower-bound to the exact $\Gamma_{1P1}$ for $\lambda \phi^4$ is given by:

$$\Gamma_{1P1}^{GEA}[\tilde{\varphi}_c] = \max_{\tilde{G}} \Gamma^A[\tilde{\varphi}_c; \tilde{G}], \quad (6.23)$$

where the auxiliary functional $\Gamma^A$ is:

$$\Gamma^A[\tilde{\varphi}_c; \tilde{G}] = -\frac{1}{2} \int_p \left[ \log \tilde{G}^{-1} \right] (p, -p) - \frac{1}{2} \int_p \left( p^2 + m_B^2 \right) \left( \tilde{G}(p, -p) + \tilde{\varphi}_c(p) \tilde{\varphi}_c(-p) \right)$$

$$- \lambda_B \int_{pqrs} \left( 3 \tilde{G}(p, q) \tilde{G}(r, s) + 6 \tilde{G}(p, q) \tilde{\varphi}_c(r) \tilde{\varphi}_c(s) + \tilde{\varphi}_c(p) \tilde{\varphi}_c(q) \tilde{\varphi}_c(r) \tilde{\varphi}_c(s) \right) \delta(p + q + r + s). \quad (6.24)$$
The optimization equation for the function $\bar{\mathcal{G}}$, obtained by functional differentiation of $\Gamma_{1FF}^{GEA}[\bar{\varphi}_c]$, can be written as

$$\bar{\mathcal{G}}^{-1}(p, q) = (p^2 + m_B^2)\delta(p + q) + 12\lambda_B \int_{rs} [G(r, s) + \bar{\varphi}_c(r)\bar{\varphi}_c(s)]\delta(p + q + r + s), \quad (6.25)$$

where $\bar{\mathcal{G}}(p, q)$ is the optimal $\bar{\mathcal{G}}$ function for an arbitrary field configuration $\bar{\varphi}_c(p)$. In order to compute the $n$-point functions, it is convenient to define the following functions

$$\theta_{m}(p, q; t_1, \ldots, t_m) \equiv \frac{\delta^m \bar{\mathcal{G}}^{-1}(p, q)}{\delta \bar{\varphi}_c(t_1) \cdots \delta \bar{\varphi}_c(t_m)}. \quad (6.26)$$

By differentiating equation (6.25), one finds that these satisfy the following linear integral equation:

$$\theta_{m}(p, q; t_1, \ldots, t_m) = k_{m}(p + q, t_1, \ldots, t_m)$$

$$- 12\lambda_B \int_{rs's'} \bar{\mathcal{G}}(r, r')\bar{\mathcal{G}}(s, s')\theta_{m}(r', s'; t_1, \ldots, t_m)\delta(p + q + r + s). \quad (6.27)$$

where the functions $k_{m}$ are to be given below. Using (6.25) and (6.27), the $\Gamma_n$ functions are given by:

$$\Gamma_2(p_1, p_2) = -\delta(p_1 + p_2)(p_1^2 + m_B^2) - 12\lambda_B \int_{pq} \bar{\mathcal{G}}(p, q)\delta(p + q + p_1 + p_2)$$

$$- \int_q \theta_{1}(p_2, q; p_1)\bar{\varphi}_c(q) + 12\lambda_B \int_{pq} \bar{\varphi}_c(p)\bar{\varphi}_c(q)\delta(p + q + p_1 + p_2), \quad (6.28)$$

$$\Gamma_3(p_1, p_2, p_3) = 48\lambda_B \int_q \bar{\varphi}_c(q)\delta(q + p_1 + p_2 + p_3) - 2\theta_{1}(p_2, p_3; p_1)$$

$$- \int_q \theta_{2}(p_3, q; p_1, p_2)\bar{\varphi}_c(q), \quad (6.29)$$

$$\Gamma_4(p_1, p_2, p_3, p_4) = 48\lambda_B \delta(p_1 + p_2 + p_3 + p_4) - 3\theta_{2}(p_3, p_4; p_1, p_2)$$

$$- \int_q \theta_{3}(p_4, q; p_1, p_2, p_3)\bar{\varphi}_c(q), \quad (6.30)$$
and for $n \geq 5$

$$
\Gamma_n(p_1, \ldots, p_n) = (1 - n) \theta_{n-2}(p_{n-1}, p_n; p_1, \ldots, p_{n-2})
- \int_q \theta_{n-1}(p_n, q; p_1, \ldots, p_{n-1}) \tilde{\varphi}_c(q). 
$$

(6.31)

For the sake of brevity, we shall often write expressions for symmetric functions of their momentum arguments, e.g. $\Gamma_n(p_1, \ldots, p_n)$, in unsymmetrized form. The fully symmetrized expressions can always be recovered by averaging over all permutations of the arguments. To make further progress, one can solve equation (6.27) by iteration.

The resulting series solution can be resumed, becoming

$$
\theta_m(p, q; t_1, \ldots, t_m) = \int_{uvw} \tilde{\delta}(p + q - u)(1 + 12\lambda_B B)^{-1}(u, v)k_m(v, t_1, \ldots, t_m). 
$$

(6.32)

where "$(1 + 12\lambda_B B)^{-1}$" is to be understood in the functional sense (so that $1 = \tilde{\delta}(u-v)$).

The function $B(u, v)$ is given by:

$$
B(u, v) = \int_{pp'qq'} \tilde{\delta}(u + p + q)\tilde{G}(p, p')\tilde{G}(q, q')\tilde{\delta}(p' + q' - v). 
$$

(6.33)

The first $k_m$'s, unsymmetrized, are given by:

$$
k_1(v, t_1) = 24\lambda_B \int_r \tilde{\varphi}_c(r)\tilde{\delta}(v + r + t_1), 
$$

(6.34)

$$
k_2(v, t_1, t_2) = 24\lambda_B \tilde{\delta}(v + t_1 + t_2)
+ 24\lambda_B \int_{pp'qq'r'r'} \tilde{G}(p, p')\tilde{G}(q, q')\tilde{G}(r, r')\theta_1(q', r'; t_1)\theta_1(p', r; t_2)\tilde{\delta}(v + p + q), 
$$

(6.35)

$$
k_3(v, t_1, t_2, t_3) = 72\lambda_B \int_{pp'qq'r'r'} \tilde{G}(p, p')\tilde{G}(q, q')\tilde{G}(r, r')
\times \theta_1(q', r'; t_1)\theta_2(p', r; t_2, t_3)\tilde{\delta}(v + p + q)
- 72\lambda_B \int_{pp'qq'r'r's's'} \tilde{G}(p, p')\tilde{G}(q, q')\tilde{G}(r, r')\tilde{G}(s, s')
$$
\[ \times \theta_1(p', q'; t_1) \theta_1(r', s'; t_2) \theta_1(q, s; t_3) \delta(v + p + r). \]  

(6.36)

For \( m \geq 3 \), \( k_m(v, t_1, \ldots, t_m) \) can be computed in terms of \( \theta_1, \ldots, \theta_{m-1} \) by the following formula:

\[
k_m(v, t_1, \ldots, t_m) =
-12 \lambda_B \sum_{n=1}^{m-1} \binom{m-1}{n} \int_{pp'qq'} D_n(p, p', q, q'; t_1, \ldots, t_n) \times \theta_{m-n}(p', q'; t_{n+1}, \ldots, t_m) \delta(v + p + q),
\]  

(6.37)

with

\[
D_n(p, p', q, q'; t_1, \ldots, t_n) \equiv \frac{\delta^n [\tilde{G}(p, p') \tilde{G}(q, q')]}{\delta \tilde{\varphi}_c(t_1) \cdots \delta \tilde{\varphi}_c(t_n)},
\]  

(6.38)

given recursively by

\[
D_n(p, p', q, q'; t_1, \ldots, t_n) = \sum_{i=0}^{n} \binom{n}{i} S_i(p, p'; t_1, \ldots, t_i) S_{n-i}(q, q'; t_{i+1}, \ldots, t_n),
\]  

(6.39)

where

\[
S_n(p, q; t_1, \ldots, t_n) \equiv \frac{\delta^n \tilde{G}(p, q)}{\delta \tilde{\varphi}_c(t_1) \cdots \delta \tilde{\varphi}_c(t_n)}
\]  

\[
= - \sum_{m=0}^{n-1} \binom{n-1}{m} \int_{pp'qq'} D_m(p, p', q, q'; t_1, \ldots, t_m) \theta_{n-m}(p', q'; t_{m+1}, \ldots, t_n),
\]  

(6.40)

for \( n \neq 0 \). The formulas above form a complete set of algebraic equations that specify \( \Gamma_n \) in terms of the optimal kernel \( \tilde{G}(p, q) \) for arbitrary \( \tilde{\varphi}_c(p) \).

Having in this fashion recursively eliminated all functional derivatives, the next step is to evaluate the \( \Gamma_n \) for a translationally invariant classical field:

\[ \tilde{\varphi}_c(p) = \varphi_c \delta(p), \]  

(6.41)

\[ \tilde{G}(p, q) = g(p) \delta(p + q) = (p^2 + \tilde{\Omega}^2)^{-1} \delta(p + q), \]  

(6.42)
where \( \bar{\Omega}^2 = m_B^2 + 12\lambda_B[I_0(\bar{\Omega}) + \varphi_c^2] \), with \( I_0(\bar{\Omega}) = \int g(p) \). It will be useful to define the following integral (for \( N > 0 \):

\[
I_{-N}(p_1, p_2, \ldots, p_N; \bar{\Omega}) = \frac{4^N N!^2}{(2N)!} \int g(q) g(q + p_1) \cdots g(q + p_N),
\]

which at zero momenta satisfies the relation \( dI_{-N}/d\bar{\Omega}^2 = -(N + 1/2)I_{-N-1} \) [22]. Thus for example,

\[
I_{-1}(p) = 2 \int g(q) g(q + p),
\]

\[
I_{-2}(p, q) = \frac{8}{3} \int g(r) g(r + p) g(r + q),
\]

\[
I_{-3}(p, q, r) = \frac{16}{5} \int g(s) g(s + p) g(s + q) g(s + r),
\]

where here and below we omit \( \bar{\Omega} \) from the argument list of \( I_{-N} \) unless it is needed for clarity. In addition we define

\[
d(p) = \frac{1}{1 + 6\lambda_B I_{-1}(p)}.
\]

For constant \( \varphi_c \), the function \( B(u, v) \) reduces to

\[
B(u, v) = \frac{1}{2} I_{-1}(v) \delta(u - v).
\]

To evaluate the \( \Gamma \)'s we first evaluate

\[
\theta_1(p, q; t_1) = 24\lambda_B \varphi_c d(t_1) \delta(p + q + t_1),
\]

\[
\theta_2(p, q; t_1, t_2) = [24 \lambda_B d(t_1 + t_2)
+ 5184 \lambda_B^3 \varphi_c^2 I_{-2}(t_1, -t_2) d(t_1) d(t_2) d(t_1 + t_2)] \delta(p + q + t_1 + t_2),
\]

\[
\theta_3(p, q; t_1, t_2, t_3) = [15552 \lambda_B^3 \varphi_c I_{-2}(-t_1, t_2 + t_3) d(t_1) d(t_2 + t_3) d(t_1 + t_2 + t_3)]
\]
\[-311040 \lambda_B^8 \phi_c^3 I_{-3}(t_1, t_1 + t_2, -t_3) d(t_1) d(t_2) d(t_3) d(t_1 + t_2 + t_3) \\
+ 3359232 \lambda_B^8 \phi_c^3 I_{-2}(-t_1, t_2 + t_3) I_{-2}(t_2, -t_3) \\
\times d(t_1) d(t_2) d(t_3) d(t_1 + t_2 + t_3)] \delta(p + q + t_1 + t_2 + t_3). \quad (6.51)

Since the first two arguments of \(\theta_n(p, q; t_1, \ldots)\) are always summed, we can write instead \(\theta_n(p + q; t_1, \ldots)\). Finally,

\[\Gamma_2(p, q) = -\delta(p + q)[p^2 + \bar{\Omega}^2 - (12\lambda_B\phi_c)^2 I_{-1}(p)d(p)], \quad (6.52)\]

\[\Gamma_3(p_1, p_2, p_3) = 48\lambda_B\phi_c\delta(p_1 + p_2 + p_3) - 2\theta_1(p_2 + p_3; p_1) - \phi_c\theta_2(p_3; p_1, p_2), \quad (6.53)\]

and

\[\Gamma_4(p_1, p_2, p_3, p_4) = 48\lambda_B\delta(p_1 + p_2 + p_3 + p_4) - 3\theta_2(p_3 + p_4; p_1, p_2) - \phi_c\theta_3(p_4; p_1, p_2, p_3). \quad (6.54)\]

As a check, at zero external momenta the \(n\)-point functions reduce to the derivatives of the GEP previously obtained.

### 6.2 Renormalization

In \(d = 4\), to renormalize the GEA, we employ the autonomous flows for the mass and coupling constant [17]:

\[m_B^2 = \frac{m_0^2 - 3\lambda_B I_0(0)}{I_{-1}(0; b)}, \quad \lambda_B = \frac{1}{12I_{-1}(0; b)}, \quad (6.55)\]

where \(I_{-1}(0; b) = 2 \int_q (q^2 + b^2)^{-2}\), \(b\) is an arbitrary finite mass scale, and \(m_0\) a finite mass parameter. In addition, with

\[\phi_c(p) = \phi_c\delta(p) + Q_c(p), \quad (6.56)\]
equation (6.21) reads

\[ \Gamma[Q_c] = \frac{1}{n!} \int_{p_1 \cdots p_n} \Gamma_n(p_1, \ldots, p_n)|_{\varphi_c} Q_c(p_1) \cdots Q_c(p_n). \] (6.57)

Thus, the coefficient of the quadratic term in the shifted field is not just \( p^2 + \bar{\Omega}^2 \), but \( \Gamma_2 \) as in (6.52), evaluated at \( \bar{\varphi}_c(p) = \phi_c \bar{\delta}(p) \). Inserting the autonomous flows, \( \varphi_c = I_{-1}^{\frac{1}{2}}(0;b) \Phi_c, \bar{\Omega}^2 = \frac{2}{3} \Phi_c^2 + O(1/I_{-1}) \), and

\[ I_{-1}(p; \bar{\Omega}) = I_{-1}(0; b) - f(p), \quad d(p) = \frac{2}{3} + \frac{2f(p)}{9I_{-1}(0; b)} + O(\frac{f^2}{f_{-1}^2}), \] (6.58)

where \( f \) is a finite function of \(|p|\) which behaves as \( \log(p^2/\bar{\Omega}^2) \) for large \(|p|\). In addition, the integrals \( I_{-N} \), for \( N > 1 \) are finite. At the vacuum, \( \Phi_c = v \), and \( \bar{\Omega}^2 = \Omega_v^2 \equiv \frac{2}{3} v^2 \); the first term on the RHS of (6.57), \( \Gamma_0 \), becomes just the GEP, times a negative volume factor, evaluated at the SSB vacuum. In addition, at the vacuum, \( \Gamma_1 = 0 \) and

\[ \Gamma_2(p, q) = -\left[ p^2 + \frac{4f(p)v^2}{9I_{-1}(0; b)} \right] \bar{\delta}(p + q). \] (6.59)

After a little algebra, the three- and four-point functions become proportional to \( I_{-1}^{\frac{3}{2}}(0; b) \) and \( I_{-1}^{\frac{2}{2}}(0; b) \), respectively, and the higher \( n \)-point functions become also infinitesimal. Thus, the GEA becomes quadratic in \( Q_c \) up to corrections of order \( O(Q_c^3/I_{-1}^{\frac{3}{2}}(0; b)) \). In \( \Gamma_2 \), the "bare" Gaussian mass squared, \( \bar{\Omega}_c^2 \), is canceled by the self-energy, the difference between these two terms being \( 4f(p)v^2/9I_{-1}(0; b) \). One interpretation of this is that the theory in the continuum limit, although it non-trivially undergoes SSB, behaves in the broken-symmetry vacuum as a free, massless theory. However, we should remark that in integrations involving \( \Gamma_2 \) one may not be able to ignore \( 4f(p)v^2/9I_{-1}(0; b) \), since the log \( p^2 \) behavior of \( f(p) \) at large momentum can lead to finite contributions.
Chapter 7  The U(1) Higgs Model

In this chapter we investigate the U(1)-Higgs model using the Gaussian Effective Action (GEA) formalism [57]. For constant classical fields (Sections 7.2 and 7.3) the results reproduce those obtained in the canonical formalism [58] and in the delta-expansion [59]. For gauge theories in general, the presence of Faddev-Popov ghosts in the path-integral restores the gauge invariance of the theory, broken by the gauge fixing term in the effective Lagrangian. In the covariant gauge, however, in the case of Abelian gauge theories, the ghosts do not interact with the gauge fields and hence can be exactly integrated out of the path-integral [52]. The remaining path-integral involves only commuting fields, and Jensen's inequality applies, leading to the GEA. For the effective action, the exact integration of the ghosts out of the path-integral means that they only contribute an additive constant term to the vacuum energy.

7.1 The Gaussian Effective Action

The Euclidean action of the theory in the covariant gauge is

\[ S = \int_x \left[ \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2\kappa} (\partial_\mu A_\mu)^2 + (D_\mu \phi)^*(D_\mu \phi) + m_B^2 \phi^* \phi + 4\lambda_B (\phi^* \phi)^2 \right], \quad (7.1) \]

where \( F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \), and the covariant derivative \( D_\mu = \partial_\mu + ie_B A_\mu \). We shall be interested in the effective action as a functional of the expectation value of the field \( \phi \). Thus, let us write first:

\[ \phi(x) = \frac{1}{\sqrt{2}} (\phi_1(x) + i\phi_2(x)), \quad (7.2) \]
with $\phi_1$ and $\phi_2$ real. Without loss of generality we can take the classical field to lie in the $\phi_1$ direction. Therefore we introduce the linear change of variables:

$$
\phi_1(x) = \phi_1'(x) + \varphi_c(x).
$$

(7.3)

Since the transformation is linear, it preserves the path-integral measure, and hence we can write (dropping the prime),

$$
\phi(x) = \frac{1}{\sqrt{2}}(\phi_1(x) + \varphi_c(x) + i\phi_2(x)).
$$

(7.4)

The action can thus be written in the following form [52]:

$$
S[A_\mu, \phi_1, \phi_2] = S_A[A_\mu] + S_{A,\phi}[A_\mu, \phi_1, \phi_2] + S_\phi(\phi_1, \phi_2),
$$

(7.5)

where

$$
S_A = \frac{1}{2} \int_x A_\mu(x) \left[ -\partial_\sigma \partial_\tau \delta_{\mu\nu} + (1 - \frac{1}{\xi}) \partial_\mu \partial_\nu \right] A_\nu(x),
$$

(7.6)

$$
S_{A,\phi} = \frac{1}{2} \int_x \epsilon^2 B(x) [\varphi_c^2 + \phi_1^2 + \phi_2^2] A_\mu(x) A_\mu(x)
$$

$$
+ \int_x \left\{ \epsilon_B A_\mu [ (\phi_1 + \varphi_c) \partial_\mu \phi_2 + \phi_2 \partial_\mu (\phi_1 + \varphi_c) + \epsilon_B^2 \varphi_c \phi_1 A_\mu A_\mu \right\},
$$

(7.7)

and $S_\phi$ given by the usual $O(2)$ $\lambda(\phi^2)^2$ action, with $\phi_1(x)$ already replaced by $\phi_1(x) + \varphi_c(x)$. The GEA is given by

$$
\Gamma^{GEA}[\varphi_c] = \max_G \left\{ \log(N) + N^{-1} \int DA_\mu D\phi_1 D\phi_2 e^{-S_G} (S_G - S) \right\},
$$

(7.8)

with

$$
N = \int DA_\mu D\phi_1 D\phi_2 e^{-S_G},
$$

(7.9)

and the quadratic test action

$$
S_G = \frac{1}{2} \int_x A_\mu G^{-1}\mu\nu A_\nu + \frac{1}{2} \int_x (\phi_1 G^{-1}_1 \phi_1 + \phi_2 G^{-1}_2 \phi_2).
$$

(7.10)
The test action is such that terms contributing only linearly to $S$ vanish upon performing the functional integrals. The GEA (up to constant terms) is then given by

$$\Gamma^{GEA} = \max_{\tilde{G}} \Gamma^A,$$

(7.11)

with the auxiliary functional

$$\Gamma^A[\tilde{\phi}_c, \tilde{G}] = \Gamma^{O(2)}[\tilde{\phi}_c, \tilde{G}_1, \tilde{G}_2] - \frac{1}{2} \Tr \ln[\tilde{G}^{-1}_{\mu\nu}(p, q)]$$

$$- \frac{1}{2} \int_p \left[ p^2 \delta_{\mu\nu} + e_B^2 \int_r (\tilde{G}_1(r, -r) + \tilde{G}_2(r, -r)) \delta_{\mu\nu} - \left(1 - \frac{1}{\xi} p_\mu p_\nu\right) \right] \tilde{G}_{\mu\nu}(p, -p)$$

$$- \frac{1}{2} e_B^2 \int_{pqrs} \tilde{\phi}_c(r) \tilde{\phi}_c(s) \tilde{G}_{\mu\mu}(p, q) \delta(p + q + r + s),$$

(7.12)

where we use Fourier amplitudes (as indicated by the tildes) and the convenient notation of Chapter 5: $f_p = 1/(2\pi)^d \int d^dp$, $\delta(p) = (2\pi)^d \delta(p)$. The optimization equations for the (optimal) $\tilde{G}$ propagators, denoted by $\tilde{G}(p, q)$ are:

$$\tilde{G}^{-1}_{\mu\nu}(p, q) = \left[ p^2 \delta_{\mu\nu} + e_B^2 \int_r (\tilde{G}_1(r, -r) + \tilde{G}_2(r, -r)) \delta_{\mu\nu} - \left(1 - \frac{1}{\xi} p_\mu p_\nu\right) \right] \delta(p + q)$$

$$+ e_B^2 \int_{pqrs} \tilde{\phi}_c(r) \tilde{\phi}_c(s) \delta(p + q + r + s) \delta_{\mu\nu},$$

(7.13)

$$\tilde{G}^{-1}_1(p, q) = \left[ p^2 + m_B^2 + e_B^2 \int_r \tilde{G}_{\mu\mu}(r, -r) \right] \delta(p + q)$$

$$+ 4\lambda_B \int_{pqrs} [3\tilde{G}_1(r, s) + \tilde{G}_2(r, s) + 3\tilde{\phi}_c(r) \tilde{\phi}_c(s)] \delta(p + q + r + s),$$

(7.14)

$$\tilde{G}^{-1}_2(p, q) = \left[ p^2 + m_B^2 + e_B^2 \int_r \tilde{G}_{\mu\mu}(r, -r) \right] \delta(p + q)$$

$$+ 4\lambda_B \int_{pqrs} [\tilde{G}_1(r, s) + 3\tilde{G}_2(r, s) + \tilde{\phi}_c(r) \tilde{\phi}_c(s)] \delta(p + q + r + s),$$

(7.15)

which results in:

$$\Gamma^{GEA}[\tilde{\phi}_c] = \Gamma^{O(2)}[\tilde{\phi}_c(p), \tilde{G}_1(p, q), \tilde{G}_2(p, q)] - \frac{1}{2} \Tr \ln[\tilde{G}^{-1}_{\mu\nu}(p, q)].$$

(7.16)
7.2 The Effective Potential

For translational invariant constant field configurations, \( \phi_c(p) = \varphi_c \delta(p) \), and the propagators become diagonal in their momentum arguments simplifying to:

\[
\tilde{G}_{\mu\nu}^{-1}(p, q) = \left[ (p^2 + \tilde{\Omega}_A^2)\delta_{\mu\nu} - (1 - \frac{1}{\xi}) p_\mu p_\nu \right] \delta(p + q),
\]

(7.17)

\[
\tilde{G}_1^{-1}(p, q) = (p^2 + \tilde{\Omega})\delta(p + q),
\]

(7.18)

\[
\tilde{G}_2^{-1}(p, q) = (p^2 + \tilde{\omega}^2)\delta(p + q),
\]

(7.19)

where the mass parameters \( \tilde{\Omega}_A, \tilde{\Omega}, \) and \( \tilde{\omega} \) are given by

\[
\tilde{\Omega}_A^2 = e^2_B [\varphi_c^2 + I_0(\tilde{\Omega}) + I_0(\tilde{\omega})],
\]

(7.20)

\[
\tilde{\Omega}^2 = m_B^2 + 4\lambda_B[3I_0(\tilde{\Omega}) + I_0(\tilde{\omega}) + 3\varphi_c^2] + e^2_B \delta(0)^{-1} \int_p \tilde{G}_{\mu\mu}(p, -p),
\]

(7.21)

\[
\tilde{\omega}^2 = m_B^2 + 4\lambda_B[I_0(\tilde{\Omega}) + 3I_0(\tilde{\omega}) + \varphi_c^2] + e^2_B \delta(0)^{-1} \int_p \tilde{G}_{\mu\mu}(p, -p),
\]

(7.22)

with \( I_0(m) = \int_p(p^2 + m^2)^{-1} \). The integral \( \int_p \tilde{G}_{\mu\mu}(p, -p) \), where

\[
\tilde{G}_{\mu\nu}(p, -p) = \frac{\delta(0)}{p^2 + \tilde{\Omega}_A^2} \left[ \delta_{\mu\nu} + (\xi - 1) \frac{p_\mu p_\nu}{p^2 + \xi \tilde{\Omega}_A^2} \right],
\]

(7.23)

can be rewritten in terms of \( I_0 \) integrals:

\[
\int_p \tilde{G}_{\mu\mu}(p, -p) = \delta(0)[(d - 1)I_0(\tilde{\Omega}_A) + \xi I_0(\sqrt{\xi} \tilde{\Omega}_A)].
\]

(7.24)

The unrenormalized effective potential finally reads:

\[
\tilde{V}_G(\varphi_c) = \frac{\delta(0)^{-1}}{2} \text{Tr} \ln[\tilde{G}_{\mu\nu}^{-1}(p, q)] + V_G^{(2)}(\varphi_c, \tilde{\Omega}, \tilde{\omega})
\]

\[
= [(d - 1)I_1(\tilde{\Omega}_A) + I_1(\sqrt{\xi} \tilde{\Omega}_A)] + V_G^{(2)}(\varphi_c, \tilde{\Omega}, \tilde{\omega})
\]

(7.25)
Thus, $\tilde{V}_G$ consists of two contributions: (1) the contribution from the now massive vector field and (2) the contribution from the two scalar fields. In examining the mass equations, the vector mass squared, $\Omega^2_A$, consists of the classical term $e_B^2 \phi^2$, plus quantum corrections from the quantum fluctuations of the scalar fields $\phi_1$ and $\phi_2$, which couple to the bare charge $e_B$. The presence of the gauge parameter $\xi$ seems unavoidable in the Gaussian approximation since the ansatz for the vector field already is not constrained to correspond to a massless vector field. However this need not to worry us. Since the exact effective action is, by construction, independent of the gauge parameter and the GEA is a rigorous lower bound, we may optimize the parameter $\xi$ over the range 0 to infinity (a negative $\xi$ results in a complex GEA.) To this end, we only need the partial derivative of $\Gamma^A$ with respect to $\xi$, or more conveniently with respect to $\xi^{-1}$, since all the other parameters have been optimized. Hence:

$$\frac{d\Gamma^{\text{GEA}}}{d\xi^{-1}} = \frac{\partial \Gamma^A}{\partial \xi^{-1}} \bigg|_{\xi^{-1}=\xi}$$  \hspace{1cm} (7.26)

$$= -\frac{1}{2} \delta(0) \int p \mu p^\nu G_{\mu\nu}(p,-p)$$  \hspace{1cm} (7.27)

$$= -\frac{1}{2} \delta(0) \int p \frac{p^2}{p^2 + \Omega^2_A} \left[ 1 + \frac{1}{\xi} \frac{p^2}{p^2 + \xi \Omega^2_A} \right]$$  \hspace{1cm} (7.28)

$$= -\frac{1}{2} \delta(0) \int p \frac{\xi p^2}{p^2 + \xi \Omega^2_A}$$  \hspace{1cm} (7.29)

Setting this expression equal to zero, the only solution for $\xi^{-1}$, consistent with dimensional regularization for $d = 4$, is $\xi = 0$, which corresponds to the Landau gauge.

### 7.3 Renormalization of the Effective Potential

To renormalize the $\tilde{V}_G$ in 4 dimensions and observe spontaneous symmetry breaking, we employ the "autonomous" renormalization scheme, following [58]. Introducing an
arbitrary finite mass scale $b$, the autonomous flows are:

$$m_B^2 = \frac{m_0^2}{I_{-1}(b)}, \quad \varphi_c^2 = I_{-1}(b)\Phi_c^2, \quad (7.30)$$

$$\lambda_B = \frac{\alpha}{I_{-1}(b)}, \quad \epsilon_B^2 = \frac{\gamma}{I_{-1}(b)}, \quad (7.31)$$

with $\alpha$ and $\gamma$ to be determined. In dimensional regularization $I_0(0) = 0$ and one can use the relation [12]

$$I_0(\Omega) = -\frac{1}{2}\Omega^2I_{-1}(b) + \frac{\Omega^2}{16\pi^2} \left[ \ln \frac{\Omega^2}{b^2} - 1 \right]. \quad (7.32)$$

As in the GEP for $O(N)$ $\lambda(\phi^2)^2$ theory one can express the derivative of the GEP as [18]:

$$\frac{d\tilde{V}_G}{d\Phi_c^2} = \frac{1}{2}(\tilde{\Omega}^2 - 8\alpha\Phi_c^2)I_{-1}(b). \quad (7.33)$$

Demanding that this be finite, and inserting the autonomous flows into the optimization equations for the mass parameters, leads to:

$$\tilde{\Omega}_A^2 = \gamma^2 \frac{1 - 32\alpha^2}{1 + 4\alpha} \Phi_c^2 + O(1/I_{-1}), \quad (7.34)$$

$$\tilde{\Omega}^2 = 8\alpha \Phi_c^2 + O(1/I_{-1}), \quad (7.35)$$

$$\tilde{\omega}^2 = \frac{32\alpha^2}{1 + 4\alpha} \Phi_c^2 + O(1/I_{-1}), \quad (7.36)$$

and the constraint

$$\gamma^2 = \frac{8\alpha(1 - 8\alpha - 64\alpha^2)}{(1 - 32\alpha^2)(3 + \xi^2)}. \quad (7.37)$$

These expressions for the masses coincide with those found in the canonical calculation [58] and the delta-expansion calculation [59] only for $\xi = 0$, which is the GEA optimal $\xi$ value as it was discussed in the previous section. Finally, the Gaussian effective potential
can be written (up to an infinite additive constant) as:

\[
\bar{V}_G(\Phi_c) = \frac{3\gamma^2(1 - 32\alpha^2)^2}{64\pi^2(1 + 4\alpha)^2} \Phi_c^4 \left[ \ln \left( \frac{\gamma(1 - 32\alpha^2)}{1 + 4\alpha} \frac{\Phi_c^2}{b^2} \right) - \frac{3}{2} \right] + V_G^{O(2)}(\Phi_c; \alpha), \tag{7.38}
\]

where \(V_G^{O(2)}(\Phi_c; \alpha)\) is given by (see eq. (5.12) of Ref.[18]):

\[
V_G^{O(2)}(\Phi_c; \alpha) = \frac{1}{2} m_0^2 \alpha \Phi_c^2 \\
+ \frac{\alpha^2 \Phi_c^4}{\pi^2\beta} \left\{ 2(\beta - 2) \left[ \ln \frac{8\alpha \Phi_c^2}{b^2} - \frac{3}{2} \right] - (\beta - 4) \ln \beta \right\}, \tag{7.39}
\]

with

\[
\beta = 3 + 16\alpha. \tag{7.40}
\]

Equations (7.34-40) describe a family of theories, for different values of \(\gamma\) and \(\alpha\), as related by the constraint relation (7.37). In Fig. 7.1 (a) we plot \(\gamma^2\) vs. \(\alpha\). In Fig. 7.1 (b) the ratios of the masses, \(\bar{\Omega}^2/\bar{\Omega}_A^2\) and \(\bar{\omega}^2/\bar{\Omega}^2\) are plotted as a function of the parameter \(\alpha\). The ratio of the bare coupling constants \(\gamma^2/\alpha\) is linear only for small \(\alpha\). This "perturbative regime" corresponds to the one-loop result of Coleman and Weinberg [8]. In this regime the scalar particle is lighter than the vector. However, the GEP result indicates the existence of a "nonperturbative regime", inaccessible to the loop expansion, in which the scalar particle is considerably heavier than the vector. This result could well have important implications for the Higgs boson mass in the Standard Model.
Fig. 7.1. The value of $\gamma^2$ (a) versus the parameter $\alpha$, as described by equation (7.37) for $\xi = 0$. In (b) the scalar to vector mass-squared ratio $\tilde{\Omega}^2/\tilde{\Omega}^2_\lambda$ (solid line) and the ratio $\tilde{\omega}^2/\tilde{\Omega}^2$ (dashed line) are plotted as functions of the parameter $\alpha$. 
Chapter 8  Conclusions and Outlook

It is important to try to improve upon the Gaussian approximation in order to test its results and implications. One way of doing so is to formulate a quasi-perturbative expansion which gives the Gaussian result in its first order [11,43,36]. A complementary approach is to continue using the variational method, but using more elaborate trial wavefunctionals.

In this thesis we have considered in detail a non-Gaussian variational calculation of the effective potential of $\lambda \phi^4$ theory. The non-Gaussian trial wavefunctional was generated by a nontrivial unitary operator $U = e^{-i\lambda B}$ acting upon a Gaussian. Expressions for the general case where given in Chapter 3, and the special case $B = \pi^3$ was explored in detail in Chapter 4.

In $0+1$ dimensions we obtained numerical results, with the following features. (1) The transformation improves the GEP upperbound on the ground-state energy of the double well potential. The improvement has the characteristics of a "second-order" correction to a "first-order" result: When the GEP is accurate the changes are small in absolute terms, but they substantially improve the percentage error. When the GEP is less accurate the changes are larger, absolutely, but they only modestly reduce the percentage error. (2) The transformation produces an effective potential whose shape differs noticeably from the GEP in the transition region from single- to double-well behavior: The "phase transition" occurs at lower $\lambda$ values and is "softer" and in several cases becomes "second-order".

In higher dimensions we have obtained the un-renormalized effective potential
for the transformation, as well as the optimization equations which determine the variational-parameter functions. We have solved these equations at the origin, and thereby obtained a correction to the Gaussian mass renormalization. Interestingly, this correction corresponds to that found in the second-order of the post-Gaussian delta expansion [36]. In 1+1 dimensions this correction allows one to compute the critical coupling constant for the SSB second-order phase transition. In higher dimensions the transformation seems to lead to an infinite $\Omega_0$ parameter in cutoff regularization. However this can remain finite in dimensional regularization. It should be possible to solve the optimization equations iteratively, as a series in powers of $\varphi_c$. The next iteration would determine the coupling-constant renormalization, necessary in 3+1 dimensions. The way is still open, therefore to obtain an explicitly renormalized effective potential from this non-Gaussian variational calculation.

In the second half of this thesis, we have discussed a covariant variational approximation for the generating functionals $W$ and $\Gamma_{1PI}$, thus removing a major disadvantage of the canonical approach, namely the noncovariance of the Hamiltonian formalism. We have shown that nonlinear transformations can be implemented as a natural generalization of the GEA through changes of field variables which leave the functional measure $D\phi$ invariant. The method effectively allows one to approximate an interacting system with a non-Gaussian test action. In the Gaussian approximation, the formalism leads naturally to the Gaussian effective action.

For the $\lambda\phi^4$ theory, we have computed the n-point proper vertex functions from the GEA at nonzero momenta and evaluated at arbitrary values of the classical field. We have applied a renormalization scheme based on the background field method [55]
to renormalize the GEA. The GEA indicates that the theory, non-trivially, undergoes SSB, but the shifted theory seems to be free and massless.

We have also applied the GEA to study the Higgs mechanism in scalar QED, in the general covariant gauge. The variational parameters of the theory can be optimized, and lead to a renormalized autonomous-like GEP. By virtue of the variational framework on which it is based, we are able to optimize the gauge parameter, which leads to the Landau gauge.

The covariant formalism discussed in this thesis, could also be applied to the study of Yang-Mills theories. In the axial gauge, the ghost fields decouple from the gauge fields. The ghost contribution to the path integral integrates out to an irrelevant constant, and the theory becomes suitable for the GEA formalism. Another possibility is to try to find nonlinear transformations which produce a determinant that cancels the Faddev-Popov determinant exactly.
References


[27] There are special cases in which the endpoint $\Omega = 0$ can give the minimum energy [31,12].


[32] The exponential form of $U$ ensures that the expectation value of $H$ retains the correct volume dependence. By requiring, further, that $U$ is unitary, one preserves the norm of the wavefunctional. If $B$ were not Hermitian then one would face the intractable problem of exactly computing the functional integral corresponding to $\langle \Psi | \Psi \rangle$.


[35] This canonical transformation will be discussed in more detail in A. Mattingly's Rice University Ph.D. Thesis, unpublished.


[40] This error figure was incorrectly given as 11.84% in Table 1 of Ref. [11].


[58] P. M. Stevenson, unpublished.