UNIVERSITY OF CALIFORNIA, SAN DIEGO

Strongly Interacting Higgs Sector Without Technicolor

A dissertation submitted in partial satisfaction of the requirements for the degree Doctor of Philosophy in Physics by

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The dissertation of Chuan Liu is approved, and it is acceptable in quality and form for publication on microfilm:

Chairman

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1994
To my wife Dan

my parents and grandparents
# Contents

Signature Page ............................................................... iii
Dedication Page .............................................................. iv
Acknowledgements ........................................................... viii
Vita ................................................................. x
Publications ............................................................. xi
Abstract ............................................................... xii

1 Introduction .................................................................. 1
   1.1 The Higgs Sector of the Minimal Standard Model .......... 1
   1.2 The Triviality Higgs Mass Bound ............................... 3
   1.3 Higher Derivative Field Theory and Indefinite Metric Quantization .... 6
   1.4 Higgs Mass Problem in Higher Derivative Scalar Field Theory .... 8
References ................................................................. 12

2 Higher Derivative Field Theories and Indefinite Metric Quantization .... 15
   2.1 Higher Derivative Oscillator ................................... 15
      2.1.1 Classical Hamiltonian ...................................... 15
      2.1.2 Quantization .................................................. 17
      2.1.3 Diagonalization .............................................. 20
      2.1.4 Ground State Wave Function ........................... 21
4.3.3 $O(N)$ Model: The Ground States ...................................... 86
4.3.4 $O(N)$ Model: The Zero Momentum Higgs States .............. 89
4.3.5 $O(N)$ Model: Two Pion States ..................................... 90

4.4 Symmetry Breaking of the Higher Derivative $O(N)$ Model ........ 91

References ................................................................. 97

5 Simulation Results and Discussions .................................. 98

5.1 Simulation Algorithms .................................................. 98
5.2 The Extraction of Physical Parameters .............................. 101

References ................................................................. 119

6 Extracting Scattering Phase Shift Using Finite Size Techniques 121

6.1 Resonance in Finite Volume .............................................. 121
6.2 Lüscher’s Formula ............................................................ 123
6.3 Integral Representation of the Zeta Function ....................... 130
6.4 Simulation Results on the Conventional $O(4)$ Model ............ 132
6.5 Lüscher’s Formula for Higher Derivative Theory .................. 134
6.6 Phase Shift for Higher Derivative Theory in $1/N$ Expansion .... 136
6.7 Phase Shift Simulations for Higher Derivative Theory ............ 137

References ................................................................. 139

7 Conclusions .............................................................. 140

References ................................................................. 143
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Abstract of the Dissertation

Strongly Interacting Higgs Sector Without Technicolor

by

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The theoretical framework for the higher derivative $O(N)$ scalar field theory is established and the theory is shown to be finite and unitary with the indefinite metric quantization. It has been shown that if the ghost states are represented by a complex conjugate pair, the theory is free of any logical inconsistencies and the ghost pair can easily evade the experimental tests.

With an underlying hypercubic lattice structure, the higher derivative $O(4)$ model is studied nonperturbatively in computer simulations. The Higgs mass bound problem is also studied within the framework of higher derivative theory. A much higher Higgs mass value in the TeV range is found with the ghost pair well-hidden in the multi-TeV range. Therefore, the higher derivative $O(4)$ model can incorporate a
strongly interacting Higgs sector without introducing more complicated structures, like technicolor, which was impossible for the conventional lattice scalar model. This means that, although the added higher derivative term is a higher dimensional operator, it changes the fundamental features (metric, energy spectrum, strength of interaction, etc.) of the theory so much that we can no longer view it as an irrelevant operator in the Lagrangian. Moreover, due to the strong interaction of the theory, it would be impossible to meaningfully define the scaling violation in the higher derivative $O(4)$ model. This implies that we will not be able to set up the Higgs mass bound in this theory unless a new nonperturbative interpretation of the Higgs mass bound is developed.
Chapter 1

Introduction

1.1 The Higgs Sector of the Minimal Standard Model

The Standard Model was first introduced in the late 1960’s to unify the electromagnetic and weak interactions \([1, 2, 3]\). The symmetry group of the Standard Model is \(SU(2)_L \times U(1)_Y\). The Minimal Standard Model corresponds to taking only one Higgs doublet in the basic representation of \(SU(2)\). The action of the Standard Model consists of several sectors which are coupled together. The action of the Higgs sector for the theory can be written as:

\[
S_H = \int d^4x \left\{ \frac{1}{2} (D_\mu \phi)\dagger (D^\mu \phi) - V(\phi) \right\},
\]

(1.1)

where \(\phi\) is a \(SU(2)\)-doublet Higgs field,

\[
\phi(x) = \begin{pmatrix}
\phi_1(x) + i\phi_2(x) \\
\phi_3(x) + i\phi_4(x)
\end{pmatrix},
\]

(1.2)

and the potential can be written as:

\[
V(\phi(x)) = -\frac{1}{2}m^2\phi(x)\dagger \phi(x) + \lambda [\phi(x)\dagger \phi(x)]^2.
\]

(1.3)
In the limit of small gauge coupling and Yukawa coupling, the Higgs sector decouples from the rest and becomes a $\phi^4$ type scalar field theory with a global symmetry $O(4)$. This limit is also referred to as the $O(4)$ limit of the Minimal Standard Model. In the Standard Model, the symmetry $SU(2)_L \times U(1)_Y$ is spontaneously broken to $U(1)_{em}$, which, in the $O(4)$ limit, corresponds to the symmetry breaking $O(4) \to O(3)$. In this limit, the Higgs mass and the vacuum expectation value $v$ are related by

$$m_H = \sqrt{8\lambda v},$$

where $\lambda$ is the renormalized coupling constant. The experimental value for $v$ is fixed to be $v \approx 250$ GeV. Therefore, the ratio $m_H/v$ also characterizes the strength of the quartic self-interaction.

The $O(4)$ limit of the Standard Model is a very interesting limit to study for two reasons. First of all, the $SU(2)$ gauge coupling is found to be very small, $g^2 \approx 0.4$. Therefore, the effects of the gauge fields on the Higgs sector is perturbative. Although the mass of the top quark remains to be determined, it is unlikely that the top mass will be much higher than 200 GeV. All the quark masses are rather light compared with the weak scale, therefore the effects of the fermion sector can also be evaluated within perturbation theory. In other words, the symmetry breaking mechanism is almost completely determined by the Higgs sector alone, plus some perturbative corrections. Secondly, on the phenomenology side, people have shown a so-called Equivalence Theorem [4] which says: when the center of mass energy $\sqrt{s}$ is much higher than the $W$ boson mass, the scattering amplitude of the $W$ bosons in the full Standard Model is equal to the scattering amplitude of the corresponding channel in the $O(4)$ model with $O(m_W/\sqrt{s})$ corrections. One of the methods in the Higgs search experiment is utilizing the $WW$ or $ZZ$ boson scattering channel. Therefore, if we consider the energy range for the Higgs search, assuming that the
Higgs mass is above the vev scale or even in the TeV range, the $O(4)$ limit would be a good approximation for the $WW$ scattering in the Standard Model. Thus, we conclude that the $O(4)$ limit of the Standard Model would be a very good laboratory for the investigation of the symmetry breaking mechanism and the mass of the Higgs particle.

1.2 The Triviality Higgs Mass Bound

Despite the successes of the Standard Model, two types of particle that are important in this model remain unconvinced by the experiments, namely, the top quark and the Higgs particle. The missing of the Higgs particle is very problematic because the Higgs plays such an important role in the spontaneous symmetry breaking which gives rise to all the masses of gauge bosons and fermions. In the past decade, there have been many efforts to put an upper bound on the Higgs mass. The early works utilized the tree level unitarity and the unitarity bound was found to be around 1 TeV [4]. Later, it was then realized that the $O(N)$ scalar field theory is a trivial field theory and this implies an upper bound on the Higgs mass [21, 22].

The triviality picture of field theory was first encountered by Landau et. al. long ago when studying the renormalization properties of Quantum Electrodynamics (QED) [20]. They discovered that, if the cutoff was brought to infinity in QED, the renormalized coupling constant of QED (the electric charge) was driven to zero logarithmically. Therefore, in order to have an interacting theory, a large but finite cutoff had to remain in the theory. Thus, QED has a built-in cutoff parameter. This implies that every quantity calculated in QED depends on this arbitrary cutoff parameter. As the energy scale gets closer and closer to the cutoff, there is more dependence on this arbitrary cutoff parameter. It seems then that we will lose the predictability of the theory. In fact, this is not a problem at all for QED. The
built-in cutoff scale, also known as the Landau ghost scale, is enormous (typically $\Lambda \sim 10^{137}$ MeV) for QED and therefore the dependence of the physical quantities on this cutoff scale is negligible. Furthermore, before this energy scale is reached, new physics (weak interactions, strong interactions) will set in and QED must be modified. However, one thing becomes clear from the above discussion, namely, we cannot calculate to arbitrary accuracy in a trivial field theory due to the existence of the arbitrary cutoff parameter.

The triviality scenario of the Higgs sector is quite similar to that of QED, except that in the Higgs sector we do not know the mass of the Higgs and the coupling constant. Therefore, the built-in cutoff for the Higgs sector could be as low as a few TeV, or as high as the Planck scale, depending on the value of the Higgs mass. Also, we do not know the nature of the new physics that lies between the built-in cutoff and the weak scale, if there is any.

The triviality of the Higgs sector can be easily seen in either perturbation theory or in the $1/N$ expansion [31] of the model. Extensive nonperturbative studies have also been performed on this model with a lattice regulator [25, 26, 27]. All nonperturbative simulation results suggest that the triviality scenario found in perturbation theory is a feature of the full theory. In these studies, the upper bound of the Higgs particle was found to be about 640 GeV under some well defined conditions which we now come to.

With the lattice regulator, the theory is made finite and the momentum cutoff is given by $\Lambda = \pi/a$. The continuum limit is achieved by taking $\Lambda \to \infty$, or equivalently, taking the lattice correlation length $\xi \to \infty$. For very large $\Lambda/m_H$, triviality of the theory forces the renormalized coupling constant $\lambda_R$ to go to zero logarithmically. Since the vacuum expectation value $v$ is fixed in physical units, this would mean the Higgs mass is also going to zero in this limit like $m_H \sim (\log(\Lambda/m_H))^{-1/2}$. 
Making a larger Higgs mass is therefore equivalent to bringing down the cutoff $\Lambda$ relative to the Higgs mass. Of course, this will generate larger cutoff dependent terms (scaling violation) in the physical scattering cross section. In the case of the lattice cutoff, the scaling violation is represented by the violation of Euclidean invariance. The old triviality Higgs mass bound was obtained by demanding that in a Goldstone scattering process (which is equivalent to $WW$ scattering in the Standard Model according to the Equivalence Theorem), there was not more than a few percent Euclidean invariance violation in the scattering cross section [26]. It is evident from the above discussion that two things are crucial to set up the triviality mass bound of the Higgs particle. First, one has to know what the scaling violation will be when a certain type of regulator is introduced. Second, one has to have a well-defined method to calculate this scaling violation for a given set of parameters. In the case of the lattice Higgs bound study, the scaling violation is the Euclidean invariance violation and the method to calculate it is perturbation theory. Perturbation theory is a valid approach for the Higgs sector, because for all Higgs mass values below the bound, the coupling is weak enough for meaningful perturbative expansion.

The old triviality Higgs mass bound was rather low because even at the upper bound value the renormalized coupling constant of the theory remains perturbative. In terms of the Higgs mass over vev ratio, $R$ is only about 3. Further increase to the Higgs mass results in a scattering amplitude with large lattice effects and can no longer represent the low energy continuum theory. Therefore, if the hypercubic lattice will not be the new physics, then the existence of a strongly interacting Higgs sector is excluded in a lattice regulated scalar field theory. There has been great concern that this finding was an artifact of the lattice regulator itself which breaks Euclidean invariance. This concern is reasonable if we consider the analogue in QCD. We know that the linear sigma model, which is nothing but the $O(4)$ model
in the broken phase, will generate the right physics of QCD at low energies (low energy theorems, PCAC, etc.). However, the corresponding ratio $m_\sigma/f_\pi \sim 7$ is much higher than in the Higgs case. Based on this analogy, technicolor models have been introduced which offers a possibility of strongly interacting Higgs sector. Due to the strong interacting nature of the technicolor at low energies, perturbation theory breaks down. Most of the analytic calculations are therefore performed using the effective chiral Lagrangian methods. A complete nonperturbative simulation of the technicolor theory including the dynamical fermions is very costly. Therefore, it would be nice to have a scalar model that can incorporate a strongly interacting Higgs sector. People have tried to perform the lattice calculation with better Euclidean invariance for the scalar models. The first significant increase of the Higgs mass bound (750 GeV) was reported [29] within the Symanzik improvement program on a hypercubic lattice structure [28]. Similar results on different lattice structures, with higher dimensional lattice operators in the interaction term, have also been reported [30].

In this thesis, I will study the scalar sector of the Minimal Standard Model and the Higgs mass problem by adding a higher derivative term in the kinetic energy of the Higgs Lagrangian. With the higher derivative term, we have a finite $O(N)$ scalar field theory interacting via a quartic coupling constant.

### 1.3 Higher Derivative Field Theory and Indefinite Metric Quantization

There have been serious concerns about the potential difficulties in higher derivative field theories [5, 6, 8, 9, 10, 11, 12, 14, 16, 17, 18, 19]. I will briefly mention some of these difficulties in this section, and the detailed study will be the subject of the subsequent chapters.
First of all, as we will see in Chapter (2), the conventional quantization procedure does not offer a meaningful theory because the spectrum is neither bounded below nor above. So, finding new ways of quantizing the higher derivative theory is necessary. One of the choices is the indefinite metric quantization \([13, 14, 11]\). By doing this the theory has a unique vacuum but, in the meantime, the positivity of the norm in the Hilbert space is lost. Therefore, one has to identify a subspace in the full Hilbert space as the physical space and maintain all the physical principles.

Unitarity is one of these principles that one would like to maintain because this is at the heart of any quantum theory for which Born’s probability description still applies. Before any meaningfully interpretation of negative probability is found, unitarity should be preserved in any physical theory. This is a big challenge for the higher derivative theories simply because the full Hilbert space is not positively normed, and negative normed states, also called ghost states, may violate unitarity. This is one of the main reasons why many people have abandoned the higher derivative field theories. However, I will demonstrate that, there could be a scenario in which the ghost particles are represented as a complex conjugate pair, and unitarity is maintained \([9, 11, 15]\). This possibility was first pointed out by T. D. Lee in the late sixties. There have been a lot of discussions on this issue and it still remains quite controversial.

Causality is another principle of the physical theory. As has been pointed out earlier by Lee \([9]\), with the complex conjugate ghost pair, only microscopic causality is violated, and macroscopically it is very difficult to detect in the experiments (see Chapter (3) for further information).
1.4 Higgs Mass Problem in Higher Derivative Scalar Field Theory

It is very interesting to study the Higgs mass bound problem in this higher derivative scalar field theory. There have always been several ways of viewing this theory. The first and most conventional way is to view it as the Pauli-Villars regulated Higgs theory [7, 11, 23, 24]. The second is to view it as a stand-alone, finite, well-defined theory with ghosts. The third is to view it as some truncated expansion of the effective low energy theory after the degrees of freedom representing the new physics have been integrated out. The original full theory probably has no ghost states, but after the truncation of the full series, the model may contain ghost excitations. Obviously, the distinction between the second and the third view is ambiguous since we do not know what the full theory should be. The first view, however, should be taken very carefully. Strictly speaking, this view is only valid in the limit of small \( m/M \) ratio, where \( m \) is the Higgs mass and \( M \) is the Pauli-Villars mass parameter. If the mass of the Higgs is getting close to the Pauli-Villars mass parameter, we have to take the second view and treat the theory as a finite theory with ghosts. In the limit of \( m/M \to 0 \), this finite theory coincides with the conventional \( O(N) \) scalar field theory with a Pauli-Villars cutoff. When the Higgs mass scale is comparable with the ghost parameter, the higher derivative field theory becomes a theory with complicated particle contents.

To study the Higgs mass bound problem in the higher derivative \( O(N) \) model, we have to answer the same two questions. First, what is the scaling violation; second, how does one calculate it?

The answer to the first question is not easy in the case of the higher derivative theory. Naively thinking, one would expect there should be some ghost effects. However, despite the negative metric ghost states in the theory, it remains unitary
and the scattering cross section of ordinary particles looks perfectly normal (see Chapter (3) for details). The only unusual effect found for the higher derivative $O(N)$ model is the violation of microscopic causality. As has been mentioned above, this type of acausal effect is extremely difficult to detect. That is to say, introducing the higher derivative terms to the theory makes the theory finite, only at the cost of violating microscopic causality, which is invisible for practical reasons. One might still worry that, in this theory, all the results will depend on the ghost mass parameter and this is some sort of scaling violation. This leads us to the second fundamental question of the problem, namely, how to calculate the scaling violations.

Obviously, if the Higgs particle remains light and the theory is still in the perturbative regime, we can do the perturbative calculation and find out how the scattering amplitude depends on the new parameter $M$. Whether to call it the scaling violation is still a question. It is some deviation from the Minimal Standard Model in the perturbative range. However, if the Higgs is heavy and the interaction is getting stronger, we will not be able to find out the scaling violation simply because we have nothing to compare with. In a strong interacting theory, we have no idea what the universal scattering amplitude will look like. In fact, we do not know how to define such a quantity meaningfully. A new nonperturbative interpretation of the Higgs mass bound therefore becomes necessary.

From the above discussion, we can see that there are several major differences between the higher derivative theory and the conventional theory on the lattice in regards to the Higgs mass bound problem. First, the scaling violation in the conventional theory with the lattice regulator is unambiguously defined, both perturbatively and nonperturbatively. Even without the help of the perturbation theory, we can quantify the violation of the Euclidean invariance meaningfully [32]. In the higher derivative case, however, the scaling violation is not well-defined, at least not
nonperturbatively. One can try to search the $M$ dependence of the theory only in perturbation theory.

Although the higher derivative theory is a finite theory, it still has infinite degrees of freedom. In order to carry out a nonperturbative simulation of the model, one must make the number of degree of freedom finite. This can be done by introducing an underlying hypercubic lattice structure to the model. The lattice spacing $a$ introduces a new short distance energy scale with the associated lattice momentum cutoff $\Lambda = \pi/a$. In order to recover the higher derivative theory in the continuum, one would have to work towards the limit $\Lambda/M \to \infty$ with a fixed ratio of $M/m_H$. In so doing, the higher derivative $O(N)$ model has the same scaling violation as the conventional model, that is, it violates Euclidean invariance. In the lattice higher derivative model, in order to recover the corresponding continuum model, one only has to eliminate the scaling violation that is associated with the lattice. For the higher derivative model on the lattice, one can view it as the conventional model on the lattice plus some so-called higher dimensional (or irrelevant) operators.

Recently, Neuberger et. al. [30] reported a new Higgs mass bound based on the systematic search in all the dimension 6 operators added to the conventional Higgs model on the $F_4$ lattice. Based on their study, they claim that the triviality Higgs mass bound is $m_H = 710 \pm 40$ GeV, and this bound value is universal in the sense that no other higher dimensional operators will change it. However, our model discussed herein contradicts their conclusion. Our model can be viewed as the conventional model plus one dimension 8 operator, which is supposed to be irrelevant according to their study. However, from all our simulation results, we can easily drive the Higgs mass value into the TeV range (see Chapter (5) for more details). We believe that the so-called “irrelevant operators” are not irrelevant at all, at least not for the Higgs mass bound problem. After all, by adding new dimension 6 irrelevant
operators, Neuberger et. al. have found a rather different bound. Therefore, the
notion of irrelevant operators is a very misleading one as far as the Higgs mass bound
problem is concerned. As we discussed above, in our model, it is impossible to set
up a precise Higgs mass bound due to the strong interaction. However, the model
is able to accommodate a Higgs particle which is heavier than the old Higgs mass
bounds with no lattice scaling violations.

My thesis is organized as follows: in Chapter 2, the quantization of the higher
derivative theory is established using indefinite metric quantization. In Chapter 3,
the higher derivative $O(N)$ model is studied within the framework of $1/N$ expansion
and the important issue of unitarity and causality are also discussed. In Chapter 4,
the lattice version of the higher derivative field theory is presented and the pos-
sibility of nonperturbative studies using Monte Carlo simulation is discussed, and
the symmetry breaking mechanism in the finite volume is studied within the Born-
Oppenheimer approximation. In Chapter 5, numerical results of the simulation are
presented and analyzed. These simulation results demonstrate that the interaction
of the higher derivative scalar field theory is much stronger than the conventional
scalar field theory. Therefore, a heavy Higgs particle in the TeV range becomes a real
possibility in the theory. Chapter 6 discusses the extraction of the resonance param-
eters of the unstable Higgs particle in the finite volume using finite size techniques.
This method, first suggested by Lüscher [33, 34], has proved to work very well for
the conventional $O(N)$ model [35, 36]. We demonstrate that this also works in the
higher derivative $O(N)$ model after appropriate adjustments. In fact, we believe this
is the only sensible way to extract the mass parameter in the simulation of a strongly
interacting theory.
References

[1] S. Weinberg, Phys. Rev. Lett. 19, (1967) 1264.

[2] A. Salam, Elementary Particle Theory, Ed., N. Svartholm, Almquist and Wiksell, 1968.

[3] S. L. Glashow, Nucl. Phys. 22, (1961) 579.

[4] B. W. Lee, C. Quigg and H. B. Thacker, Phys. Rev. D16, (1977) 1519.

[5] M. Ostrogradski, Mem. Ac. St. Petersbourg 4 (1850) 385.

[6] B. Podolski, Phys. Rev. 62 (1942) 68; B. Podolski and P. Schwed, Rev. Mod. Phys. 20 (1948) 40.

[7] W. Pauli and F. Villars, Rev. Mod. Phys. 21 (1949) 434

[8] A. Pais and G. E. Uhlenbeck, Phys. Rev. 79 (1950) 145

[9] T. D. Lee and G. C. Wick, Nucl. Phys. B 9 (1969) 209; Phys. Rev. D 2 (1970) 1033.

[10] R. E. Cutkosky, P. V. Landshoff, D. I. Olive and J. C. Polkinghorne, Nucl. Phys. B12 (1969) 281.

[11] K. Jansen, J. Kuti, C. Liu Phys. Lett. B 309 (1993) 119.

[12] D. G. Boulware and D. J. Gross, Nucl. Phys. B233 (1983) 1.
[13] W. Pauli, Rev. Mod. Phys. 15 (1943) 175.

[14] J. Z. Simon, Phys. Rev. D41 (1990) 3720.

[15] J. Kuti and C. Liu, to be published.

[16] A. A. Slavnov, Nucl. Phys. B31 (1971) 301.

[17] S. W. Hawking, Quantum field theory and quantum statistics, eds. I. A. Batalin et al. (1987) p. 129.

[18] K. S. Stelle, Phys. Rev. D16 (1977) 953.

[19] E. Tomboulis, Phys. Lett. B97 (1980) 77.

[20] L. D. Landau, A. A. Abrikosov and I. M. Khalatnikov, Doklady Akad. Nauk USSR 95 (1954) 1177.

[21] L. Maiani, G. Parisi and R. Petronzio, Nucl. Phys. B136 (1978) 115.

[22] R. Dashen and H. Neuberger, Phys. Rev. Lett. 50 (1983) 1897.

[23] K. Jansen, J. Kuti, C. Liu Phys. Lett. B309 (1993) 127.

[24] C. Liu, K. Jansen and J. Kuti, Nucl. Phys. B 34 (Proc. Suppl.), (1994) 635.

[25] J. Kuti, L. Lin, Y. Shen, Nucl. Phys. (Proc. Suppl.) B 4 (1988) 397; Phys. Rev. Lett. 61 (1988) 678.

[26] M. Lüscher and P. Weisz, Phys. Lett. B212 (1988) 472.

[27] A. Hasenfratz et al., Nucl. Phys. B317 (1989) 81.

[28] K. Symanzik, Nucl. Phys. B226 (1983) 187.
[29] M. Göckeler, H. Kastrup, T. Neuhaus and F. Zimmermann, Nucl. Phys. (Proc. Suppl.) B26 (1992) 516.

[30] U. M. Heller, H. Neuberger and P. Vranas, Nucl. Phys. B405 (1993) 557.

[31] M. B. Einhorn, Nucl. Phys. B246 (1984) 75. M. B. Einhorn and D. N. Williams, Phys. Lett. B211 (1988) 4570.

[32] C. B. Lang, Phys. Lett. B229 (1989) 97; Nucl. Phys. B (Proc. Suppl.) 17 (1990) 665.

[33] M. Lüscher, Nucl. Phys. B354 (1991) 531; Nucl. Phys. B364 (1991) 237.

[34] M. Lüscher, U. Wolff, Nucl. Phys. B339 (1990) 222.

[35] F. Zimmermann, J. Westphalen, M. Göckeler and H. A. Kastrup, Nucl. Phys. B (Proc. Suppl.) 30 (1993) 879.

[36] F. Zimmermann, J. Westphalen, M. Göckeler and H. A. Kastrup, Nucl. Phys. B (Proc. Suppl.) 34 (1994) 566.
Chapter 2

Higher Derivative Field Theories and Indefinite Metric Quantization

2.1 Higher Derivative Oscillator

2.1.1 Classical Hamiltonian

Many important features of higher derivative field theories can be illustrated by their simple quantum mechanical counterparts. As an example, let us first study a higher derivative oscillator [8] given by the following Lagrangian

\[
L = \frac{1}{2} (1 + 2\frac{m^2}{M^2}\cos 2\Theta)\dot{x}^2 - \left(\frac{\cos 2\Theta}{M^2} + \frac{m^2}{2M^4}\right)\ddot{x}^2 + \frac{1}{2M^4} x^2 - \frac{m^2}{2} x^2. \tag{2.1}
\]

This Lagrangian describes a simple harmonic oscillator of frequency \( m \) with second and third derivative terms added. For simple interpretation of the spectrum, the coefficients of the derivative terms are given in terms of \( M \) and \( \Theta \); the only restrictions imposed are \( m/M < 1 \) and \( 0 < \Theta < \pi/2 \). With the higher derivative terms added, this Lagrangian produces new features that are not present in the conventional theory. Classically, one can look at the time evolution of the position \( x(t) \) which is a solution of the corresponding Euler-Lagrange equation

\[
(1 + 2\frac{m^2}{M^2}\cos 2\Theta)\frac{d^2x}{dt^2} + \left(\frac{2\cos 2\Theta}{M^2} + \frac{m^2}{M^4}\right)\frac{d^4x}{dt^4} + M^{-4}\frac{d^6x}{dt^6} + m^2 x = 0. \tag{2.2}
\]
Some of the new features of the higher derivative theory already appear at the classical level. For example, in order to specify the solution, one has to know more initial conditions than in the usual theory. In this particular example, one needs to know \( x^{(n)}(0), n = 0, 1, \cdots, 5 \) to specify a unique solution, where \( x^{(n)} \) denotes the \( n \)-th time derivative of the variable \( x \). This in fact tells us that the higher derivative theory has more degrees of freedom than the conventional theory. Another new feature is that there are runaway solutions to this classical equation of motion [2].

The Hamiltonian of a higher derivative Lagrangian was worked out long time ago by Ostrogradsky [1]. In the Hamiltonian formalism, new degrees of freedom show up explicitly due to the higher derivative terms. In this particular example, there are three independent coordinates and their corresponding conjugate momenta, given by

\[
\begin{align*}
q_1 &= x, \quad q_2 = \dot{x}, \quad q_3 = \ddot{x}, \\
p_1 &= \frac{1}{2} (1 + 2 \frac{m^2}{M^2} \cos 2\Theta) \dot{x} + \left( \frac{\cos 2\Theta}{M^2} + \frac{m^2}{2M^2} \right) x + \frac{1}{2M^4} x, \\
p_2 &= -\left( \frac{\cos 2\Theta}{M^2} + \frac{m^2}{2M^2} \right) \ddot{x} - \frac{1}{2M^4} \dddot{x}, \\
p_3 &= \frac{1}{2M^4} \dddot{x}.
\end{align*}
\]

Notice that \( p_1 \) is not proportional to \( \dot{x} \) any more. Instead, both \( \dot{x} \) and \( \ddot{x} \) become independent variables. In terms of these variables the Hamiltonian reads

\[
H = p_1 q_2 + p_2 q_3 + \frac{M^4}{2} p_3^2 - \frac{1}{2} (1 + 2 \frac{m^2}{M^2} \cos 2\Theta) q_2^2 + \left( \frac{\cos 2\Theta}{M^2} + \frac{m^2}{2M^2} \right) q_3^2 + \frac{m^2}{2} q_1^2.
\]

The classical equation of motion can be written out in the Hamiltonian form

\[
\begin{align*}
\frac{d}{dt} q_i &= \frac{\partial H}{\partial p_i}, \\
\frac{d}{dt} p_i &= -\frac{\partial H}{\partial q_i}.
\end{align*}
\]
where $i$ runs from 1 to 3. It is easy to verify that the Hamilton equations of motion are equivalent to the Euler-Lagrange form, once we have expressed everything in terms of $q_1(t) \equiv x(t)$ and its time derivatives. Note, however, that this Hamiltonian does not look like the conventional Hamiltonian at all. The limit of small $m/M$ is a singular limit, and we will not be able to recover the standard oscillator Hamiltonian by taking this limit.

### 2.1.2 Quantization

Let us now try to quantize this Hamiltonian with the conventional canonical method. We will treat $q_1$, $q_2$ and $q_3$ as independent variables and they have the usual commutator with the corresponding momenta

$$[q_i, p_j] = i\delta_{ij}, \quad i, j = 1, 2, 3, \quad (2.6)$$

with other commutators vanishing. This already says something unusual about this quantum theory, namely that the position of a particle and its velocity are independent variables and can be measured simultaneously; while in conventional quantum mechanics they form a conjugate pair and cannot be measured simultaneously. In the higher derivative theory, it is the quantity $p_1$ that cannot be simultaneously measured with $q_1$. From the expression of $p_1$, it implies that the measurement of $x$ together with $\dddot{x}$, $\dot{x}$ together with $\dddot{x}$ and $\dddot{x}$ together with $\dddot{x}$ are impossible.

It is not very easy to see that the quadratic Hamiltonian in Equation (2.4) still represents the oscillator spectrum. In fact, using a linear transformation, the quadratic part of the Hamiltonian can be diagonalized exactly

$$H_0 = (a^\dagger a + \frac{1}{2})m - (b^\dagger b + \frac{1}{2})\mathcal{M} + (c^\dagger c + \frac{1}{2})\overline{\mathcal{M}}, \quad (2.7)$$

with $\mathcal{M} = Me^{i\Theta}$ and $\overline{\mathcal{M}} = Me^{-i\Theta}$. The creation and annihilation operators ap-
appeared in the above equation are linear combinations of \( q_i \) and \( p_i \) and satisfy the following standard commutation relations:

\[
[a, a^\dagger] = [b, b^\dagger] = [c, c^\dagger] = 1. \tag{2.8}
\]

The other commutators all vanish. This type of spectrum has many problems \cite{8}. It is not bounded below, not even the real part. Therefore, no ground state exists in this theory. This unboundedness is a very common feature to all higher derivative quantum theories. It is a direct reflection of the the “wrong sign” in front of one of the quadratic terms in the Hamiltonian. One way of dealing with these problems is to try another quantization procedure and this is where indefinite metric quantization \cite{3, 4, 7} comes in.

The idea of using negative metric in the quantization procedure was introduced long ago, especially for the quantization of gauge fields \cite{7}. In this framework, the full Hilbert space is too large for physical interests. It contains negative normed states which are necessary for the consistent quantization. The negative normed states must be removed from the physical subspace to maintain the probability interpretation of the theory. We will apply the same idea here \cite{5}.

First, notice that by appropriate scaling: \( q_1 \rightarrow \rho q_1 \) and \( q_2 \rightarrow q_2/\rho \), with \( \rho^2 = 1 + 2m^2 \cos 2\Theta/M^2 \) and by the change \((p_2, q_2) \rightarrow (-q_2, p_2)\), we can rewrite the Hamiltonian into the following form

\[
H = p_1 p_2 - \frac{p_2^2}{2} + \frac{p_3^2}{2} - \frac{M^2}{\rho} q_2 q_3 + \frac{1}{2} (m^2 + 2M^2 \cos 2\Theta) q_3^2 + \frac{1}{2} m^2 \rho^2 q_1^2. \tag{2.9}
\]

Now make the substitution

\[
p_2 \rightarrow +i p_2, \quad q_2 \rightarrow -i q_2. \tag{2.10}
\]

This will not change the commutator of \( q_2 \) and \( p_2 \) and we may write the Hamiltonian
as

\[ H = \frac{1}{2} P_1^2 + \frac{1}{2} P_2^2 + \frac{1}{2} P_3^2 + \frac{1}{2} Q^T M Q, \tag{2.11} \]

where the P’s and Q’s are related to original variables by the following table

\[ P_1 = p_1, \quad P_2 = p_2 + ip_1, \quad P_3 = p_3, \]

\[ Q_1 = q_1 - iq_2, \quad Q_2 = q_2, \quad Q_3 = q_3. \tag{2.12} \]

We have used the matrix notation \( Q \) and \( Q^T \) and the mass matrix \( M \) is

\[
M = \begin{pmatrix}
m^2 \rho^2 & im^2 \rho^2 & 0 \\
im^2 \rho^2 & -m^2 \rho^2 & i \frac{M^2}{\rho} \\
0 & i \frac{M^2}{\rho} & m^2 + 2M^2 \cos 2\Theta
\end{pmatrix}. \tag{2.13}
\]

Negative metric quantization corresponds to demanding that the \( p \)’s and \( q \)’s are hermitian, so the Hamiltonian (2.11) itself is not hermitian. Rather, it is self-adjoint with respect to a metric operator \( \eta \) satisfying

\[ \eta H^\dagger \eta = H, \]

\[ \eta q_2 \eta = -q_2, \quad \eta p_2 \eta = -p_2, \tag{2.14} \]

\[ \eta^2 = 1, \quad \eta = \eta^\dagger. \]

In this indefinite Hilbert space, the inner product of any two states, \( |\psi\rangle \) and \( |\phi\rangle \), is defined to be \( \langle \psi | \eta | \phi \rangle \). It is easy to show that the expectation value of any self-adjoint operator is real in any states. Therefore, the expectation value of the Hamiltonian in any state is real, although the eigenvalues of the Hamiltonian may
be complex. This immediately implies that the complex energy eigenstates have zero norm. The dynamics of any state vector are still governed by the Schrödinger equation

\[ i \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle. \]  

(2.15)

It is easy to show that the norm of a state is still preserved under time evolution.

\textbf{2.1.3 Diagonalization}

We can now perform transformation of the variables \( Q \) and \( P \) according to a “rotation” \( A \)

\[ \tilde{Q} = AQ, \quad \tilde{P} = AP, \]

\[ A^T A = AA^T = 1, \]  

(2.16)

and diagonalize the mass matrix \( M \). The eigenvalues of this matrix are simply given by \( m^2, M^2 = M^2 e^{2i\Theta} \) and \( \overline{M}^2 = M^2 e^{-2i\Theta} \). This is why we chose complicated parametrization of the Lagrangian. Therefore, we can define the creation and annihilation operators as

\[ a^{(\pm)} = \frac{1}{\sqrt{2}} (\sqrt{m\tilde{Q}_1} \pm \frac{i\tilde{P}_1}{\sqrt{m}}), \]

\[ b^{(\pm)} = \frac{1}{\sqrt{2}} (\sqrt{M\tilde{Q}_2} \pm \frac{i\tilde{P}_2}{\sqrt{M}}), \]  

(2.17)

\[ c^{(\pm)} = \frac{1}{\sqrt{2}} (\sqrt{\overline{M}\tilde{Q}_3} \pm \frac{i\tilde{P}_3}{\sqrt{\overline{M}}}). \]
These operators satisfy the standard commutation relation

\[ [a^(-), a^+] = [b^(-), b^+] = [c^(-), c^+] = 1, \]  

(2.18)

and the Hamiltonian has the standard oscillator form

\[ H = (a^+ a^-) + \frac{1}{2} m + (b^+ b^-) + \frac{1}{2} M + (c^+ c^-) + \frac{1}{2} \bar{M}. \]  

(2.19)

The ground state is defined to be the state which is simultaneously annihilated by \( a^(-), b^(-) \) and \( c^(-) \). We assume that the ground state is positively normed to 1. Negative metric is seen from the adjoint relations among the creation and annihilation operators

\[ \eta a^(-)^\dagger \eta = a^+, \quad \eta b^(-)^\dagger \eta = c^+, \quad \eta c^(-)^\dagger \eta = b^+. \]  

(2.20)

We can then build up our full Hilbert space by applying the various creation operators to the ground state. The eigenvalues of the Hamiltonian can, in general, be complex if the complex ghost pair is not evenly excited. All the eigenstates with complex energy have zero norms. This is a common feature for all self-adjoint Hamiltonians. The excited states are constructed and normalized according to

\[ |n_a, n_b, n_c\rangle = \frac{(a^+)^{n_a} (b^+)^{n_b} (c^+)^{n_c}}{\sqrt{n_a!} \sqrt{n_b!} \sqrt{n_c!}} |0, 0, 0\rangle, \]

\[ \langle n'_a, n'_b, n'_c | \eta | n_a, n_b, n_c \rangle = \delta_{n_a,n'_a} \delta_{n_b,n'_b} \delta_{n_c,n'_c}. \]

(2.21)

### 2.1.4 Ground State Wave Function

We can work out the coordinate space wavefunction for the ground state by substituting the old variables. We get

\[ \Psi(q_1, q_2, q_3) = N_{000} \exp\left(-\frac{m}{2} \frac{1 - \frac{m^3}{M^2} \sin 5\Theta + \frac{m^3}{M^2} \sin 3\Theta}{1 - 2 \frac{m^2}{M^3} \cos 2\Theta + \frac{m^2}{M^3}} q_1^2 \right) \]
\[ - \frac{m}{2} \frac{(\frac{m}{M} + \frac{M}{m}) \sin \Theta - 1}{1 - 2 \frac{m^2}{M^2} \cos 2\Theta + \frac{m^4}{M^4}} q_2^2 \]

\[ - \frac{m}{2} \frac{\left( \frac{m^4}{M^4} \right) \frac{1 - \frac{M^3 \sin 5\Theta}{m^3 \sin 2\Theta} + \frac{M^3 \sin 3\Theta}{m^3 \sin 2\Theta}}{1 - 2 \frac{m^2}{M^2} \cos 2\Theta + \frac{m^4}{M^4}} q_3^2 \]

\[ + \frac{m}{M^3} \frac{1 - \frac{m \sin 3\Theta}{M \sin 2\Theta} - \frac{m^3 \sin \Theta}{M^3 \sin 2\Theta}}{1 - 2 \frac{m^2}{M^2} \cos 2\Theta + \frac{m^4}{M^4}} (iq_1 q_2) \]

\[ - \frac{m^3}{M^3} \frac{1 - \left( \frac{m}{M} + \frac{M}{m} \right) \frac{\sin \Theta}{\sin 2\Theta}}{1 - 2 \frac{m^2}{M^2} \cos 2\Theta + \frac{m^4}{M^4}} (iq_2 q_3) \]

\[ + \frac{m^3}{M^3} \frac{1 - \left( \frac{m}{M} + \frac{M}{m} \right) \frac{\sin \Theta}{\sin 2\Theta}}{1 - 2 \frac{m^2}{M^2} \cos 2\Theta + \frac{m^4}{M^4}} (q_1 q_3) \].

In order for the ground state to be normalizable, some constraints must be put on the parameters $M/m$ and $\Theta$. First of all, the normalization condition is somewhat different in the case of indefinite metric quantization. The condition is

\[ \langle 0 | \eta | 0 \rangle \equiv \langle 0 | \eta | q_1, q_2, q_3 \rangle \langle q_1, q_2, q_3 | 0 \rangle = 1, \]

where we have omitted the sum (integration) over the $q_i$'s. The ground state wave function given above is just $\langle q_1, q_2, q_3 | \eta | 0 \rangle$. Therefore, due to the existence of $\eta$ which flips the sign of $q_2$, the normalization condition for the ground state wave function is written as

\[ \int dq_1 dq_2 dq_3 \Psi^*(q_1, -q_2, q_3) \Psi(q_1, q_2, q_3) = 1. \]

Now we can write down the sufficient condition for this Gaussian type integral to converge. Since the quantity $1 - 2(m^2/M^2) \cos 2\Theta + m^4/M^4$ is always positive, the
condition for normalizability reduces to the following

\[ f_0(m/M, \Theta) > 0, \quad f_0(M/m, \Theta) > 0, \]

\[ f_1(m/M, \Theta) > 0, \quad f_0(m/M, \Theta)f_0(M/m, \Theta) - f_1(m/M, \Theta)^2 > 0, \]

\[ f_0(x, \Theta) = 1 - x^3 \frac{\sin 5\Theta}{\sin 2\Theta} + x^5 \frac{\sin 3\Theta}{\sin 2\Theta}, \]

\[ f_1(x, \Theta) = (x + \frac{1}{x}) \frac{\sin \Theta}{\sin 2\Theta} - 1. \quad (2.25) \]

The condition \( f_1(m/M, \Theta) > 0 \) is equivalent to the condition \( 0 < \Theta < \pi/2 \). In order to fulfill the other conditions the parameter pair \((m/M, \Theta)\) has to be in some range. In Figure (2.1), the function \( f_0(x, \Theta)f_0((1/x), \Theta) - f_1(x, \Theta)^2 \) is plotted as a function of \( \Theta \) for some values of \( x = m/M \). Since this combination is symmetric with respect to the change \( x \to (1/x) \), it is sufficient to study the behavior in the parameter range \( 0 < x < 1 \). It is seen from this figure that for any value of the parameter \( x \), there exists a critical value \( \Theta_c(x) \) below which the ground state normalizability is preserved. In Figure (2.2), this function is plotted in the whole range \( 0 < x < 1 \). As a result, if we restrict the angle \( \Theta \) to be less than about \( \pi/3 \), the ground state wave function is normalizable for all values of \( m/M \).

It is useful to have the expression of \( q_1 \) in terms of the creation and annihilation operators:

\[ q_1 = \frac{a^{(+)}}{\sqrt{2m} \sqrt{(1 - \frac{m^2}{M^2})(1 - \frac{m^2}{M^2})}} + \frac{b^{(+)}}{\sqrt{2M} \sqrt{(1 - \frac{m^2}{M^2})(-1 + \frac{M^2}{M^2})}} \]

\[ + \frac{c^{(+)}}{\sqrt{2M} \sqrt{(1 - \frac{M^2}{M^2}(-1 + \frac{M^2}{M^2})}}. \quad (2.26) \]
Figure 2.1: The expression $f_0(x, \Theta)f_0((1/x), \Theta) - f_1(x, \Theta)^2$, as given in the above equations for various values of $x$ is plotted versus the variable $2\Theta/\pi$. This combination is always positive for a given value of $x$ as long as $\Theta$ is less than some critical value $\Theta_c(x)$.

This concludes our discussion of the higher derivative oscillator.

Note that, if we have an extra term $-\lambda_0 x^4$ in the starting Lagrangian, then our Hamiltonian would consist of two parts, $H = H_0 + H_1$, where $H_0$ is just the oscillator Hamiltonian discussed above and $H_1 = \lambda_0 q_1^4$ with $q_1$ given by Equation (2.26).

Thus, the oscillator gives us a good starting point for perturbation theory.
Figure 2.2: The critical value $\Theta_c(x)$ is plotted as a function of $x = m/M$. All the parameter pairs $(x, \Theta)$ below this curve will ensure the normalizability of the ground state wave function.

2.1.5 Euclidean Path Integral

Now let us evaluate the partition function of the higher derivative theory defined by

$$Z = \text{Tr} e^{-\beta H} \equiv \sum_s \langle \bar{s} | \eta e^{-\beta H} | s \rangle,$$

(2.27)

where the summation is over all states $|s\rangle$ such that they are complete:

$$\sum_s |s\rangle \langle s| \eta = 1.$$

(2.28)

One convenient choice for the states is $|q_1, q_2, q_3\rangle$. Then one can make use of the derivative forms of the momentum operators and derive a path integral form for the
partition function, just like in the usual theory. First one has to slice the Euclidean time $\beta$ into small intervals and, then, the partition function is written in terms of the integration of the intermediate positions. This path integral form of the partition function is exactly the Euclidean path integral that one would naively write down when not concerned with the canonical quantization procedure \[6, 10\]

$$
Z[J] = \int Dq \exp \left( -\int_0^\beta d\tau L_E[q(\tau)] + J(\tau)q(\tau) \right),
$$

$$
L_E = \frac{1}{2}\left(1 + \frac{m^2}{M^2} \cos 2\Theta\right)\dot{q}^2 + \left(\frac{\cos 2\Theta}{M^2} + \frac{m^2}{2M^4}\right)\ddot{q}^2 + \frac{1}{2M^4}\dddot{q}^2 + \frac{m^2}{2q^2}. \quad (2.29)
$$

The Euclidean propagator of the variable $q(\tau)$ can be found by differentiating the partition functional with respect to the external source $J(\tau)$. In Fourier space, it is given by

$$
D_E(E) = \frac{M^4}{(E^2 + m^2)(E^2 + M^2\cos 2\Theta)(E^2 + M^2\cos 2\Theta)}. \quad (2.30)
$$

The multiple pole structure in the propagator is a manifestation of the spectrum of the theory. As can be seen clearly, the poles are located exactly at three types of energy gaps of the theory.

There is a big difference here in the higher derivative theory as compared with the usual theory. The Minkowski path integral \[5, 9\] is not well defined. In fact, due to the complex ghost energy, it has runaway modes at large temporal separation. Also, we cannot do a wick rotation from the Euclidean to the Minkowski because of the complex ghost pole on the first sheet. We should emphasize that the Euclidean path integral is still well defined. This is the object that we will be using in our numerical simulation of the theory. Also, the Euclidean path integral in principle contains all the information about the higher derivative theory. By measuring the Euclidean propagator of the theory, one can extract the energy excitations of the
higher derivative theory and, hence, the eigenvalues of the Hamiltonian.

2.2 Higher Derivative Free Field Theory

Having discussed the quantum mechanical oscillator, let us now turn to the simplest higher derivative field theory, free field theory. Since most of the procedures are quite similar to the quantum mechanical case, we will be very brief in this section. Consider the one component higher derivative scalar field theory parametrized by the Lagrangian

\[ \mathcal{L} = \frac{1}{2} \phi(x)(-\Box - m_0^2)(1 + \frac{\Box}{M^2})(1 + \frac{\Box}{M^2})\phi(x), \quad (2.31) \]

where the \( \Box \) is the Minkowski d’Alambert operator. The Hamiltonian density can be obtained in the same way as in the quantum mechanical example

\[ \mathcal{H} = \pi_1 \phi_2 + \pi_2 \phi_3 + \frac{M^4}{2} \pi_3^2 - \frac{1}{2} \phi_2(\rho_1 - 2\rho_2 \nabla^2 + 3\rho_3 \nabla^4)\phi_2 + \frac{1}{2} \phi_3(\rho_2 - 3\rho_3 \nabla^2)\phi_3 \]

\[ + \frac{1}{2} \phi_1(-\rho_1 \nabla^2 + \rho_2 \nabla^4 - \rho_3 \nabla^6 + m_0^2)\phi_1. \quad (2.32) \]

Again, we can interchange the role of \( \pi_2 \) and \( \phi_2 \), which amounts to \( \phi_2 \rightarrow \pi_2 \) and \( \pi_2 \rightarrow -\phi_2 \). We also impose negative metric on \( \pi_2 \) and \( \phi_2 \) by doing the substitution \( \phi_2 \rightarrow -i \phi_2 \) and \( \pi_2 \rightarrow +i \pi_2 \), and after these changes our Hamiltonian density is,

\[ \mathcal{H} = i \pi_1 \pi_2 + \frac{1}{2\rho_3} \pi_3^2 + \frac{1}{2} \pi_2(\rho_1 - 2\rho_2 \nabla^2 + 3\rho_3 \nabla^4)\pi_2 + \frac{1}{2} \phi_3(\rho_2 - 3\rho_3 \nabla^2)\phi_3 \]

\[ + \frac{1}{2} \phi_1(-\rho_1 \nabla^2 + \rho_2 \nabla^4 - \rho_3 \nabla^6 + m_0^2)\phi_1 + i \phi_2 \phi_3. \quad (2.33) \]

Negative metric quantization then corresponds to making \( \phi_i, i = 1, 2, 3 \) and \( \pi_i, i = 1, 2, 3 \) hermitian operators. Then the Hamiltonian itself is not hermitian but still self-adjoint with respect to the negative metric \( \eta \) which flips the sign of \( \pi_2 \) and \( \phi_2 \).
We have
\[ \eta H^\dagger \eta = H. \] (2.34)

Introducing the Fourier modes
\[ \phi_i(x) = \bar{\phi}_i + \sum_{k>0} \frac{1}{\sqrt{V}} [\phi_{i,k} e^{ik \cdot x} + \phi_{i,k}^* e^{-ik \cdot x}], \] (2.35)
where the index \( i \) runs from 1 to 3. We can also write the similar expression for \( \pi_i \)
\[ \pi_i(x) = \bar{\pi}_i + \sum_{k>0} \frac{1}{\sqrt{V}} [\pi_{i,k} e^{-ik \cdot x} + \pi_{i,k}^* e^{ik \cdot x}]. \] (2.36)

To ensure basic commutation relations, we must have
\[ [\phi_{i,k}, \pi_{j,k'}] = i \delta_{ij} \delta_{kk'}, \quad [\bar{\phi}_i, \pi_j] = i \delta_{ij}. \] (2.37)

We can then write the Hamiltonian as
\[
H = \frac{1}{V} (i \bar{\pi}_1 \bar{\pi}_2 + \frac{\bar{\pi}_3 \pi_3}{2\rho_3} + \frac{\rho_2}{2} \bar{\pi}_2^2) + V \left( \frac{\rho_2}{2} \bar{\pi}_3^2 + \frac{m^2}{2} \bar{\phi}_1^2 + i \bar{\phi}_2 \pi_3 \right) \\
+ \sum_{k>0} i (\pi_{1,k} \pi_{2,k}^* + \bar{\pi}_{1,k} \bar{\pi}_{2,k}) + \frac{\pi_{3,k} \bar{\pi}_{3,k}}{\rho_3} + (\rho_1 + 2 \rho_2 \kappa^2 + 3 \rho_3 \kappa^4) \pi_{2,k} \bar{\pi}_{2,k} \\
+ (\rho_1 \kappa^2 + \rho_2 \kappa^4 + \rho_3 \kappa^6 + m_0^2) \phi_{1,k} \phi_{1,k}^* + (\rho_2 + 3 \rho_3 \kappa^2) \phi_{3,k} \phi_{3,k}^* \\
+ i (\phi_{2,k} \phi_{3,k}^* + \phi_{2,k}^* \phi_{3,k}). \] (2.38)

After some rescaling of the variables we can bring the Hamiltonian into similar form as in the quantum mechanical oscillator case
\[ H = H_0 + \sum_{k>0} \pi_{ik}^* \pi_{ik} + \phi_{ik}^* M_{ij} \phi_{jk}. \] (2.39)
We then perform the same "rotation" transformation as in the oscillator case, and then the above Hamiltonian is diagonalized to

$$H = H_0 + \sum_{\mathbf{k} > 0} \Pi^*_\mathbf{ik} \Pi_\mathbf{ik} + \Phi^*_\mathbf{ik} \omega^2_{\mathbf{ik}} \Phi_{\mathbf{jk}}, \quad (2.40)$$

where the frequency $\omega_{0\mathbf{k}} = \sqrt{m^2_0 + \mathbf{k}^2}$, $\omega_{1\mathbf{k}} = \sqrt{\mathcal{M}^2 + \mathbf{k}^2}$ and $\omega_{2\mathbf{k}} = \sqrt{\mathcal{M}^2 + \mathbf{k}^2}$. The creation and annihilation operators are given by

$$a^{(-)}_{i\mathbf{k}} = \frac{1}{\sqrt{2}} \left( \sqrt{\omega_{1\mathbf{k}}} \Phi_{i\mathbf{k}} + \frac{i}{\sqrt{\omega_{1\mathbf{k}}}} \Pi^*_\mathbf{ik} \right),$$

$$a^{(+)}_{i\mathbf{k}} = \frac{1}{\sqrt{2}} \left( \sqrt{\omega_{1\mathbf{k}}} \Phi_{i\mathbf{k}} - \frac{i}{\sqrt{\omega_{1\mathbf{k}}}} \Pi^*_\mathbf{ik} \right),$$

$$a^{(-)}_{i-\mathbf{k}} = \frac{1}{\sqrt{2}} \left( \sqrt{\omega_{3\mathbf{k}}} \Phi^*_i \mathbf{k} + \frac{i}{\sqrt{\omega_{3\mathbf{k}}}} \Pi_{i\mathbf{k}} \right),$$

$$a^{(+)}_{i-\mathbf{k}} = \frac{1}{\sqrt{2}} \left( \sqrt{\omega_{3\mathbf{k}}} \Phi^*_i \mathbf{k} - \frac{i}{\sqrt{\omega_{3\mathbf{k}}}} \Pi_{i\mathbf{k}} \right), \quad (2.41)$$

with $i = 1, 2, 3$. The Hamiltonian finally looks like

$$H = \sum_{\mathbf{k}} (a^{(+)}_{i\mathbf{k}} a^{(-)}_{i\mathbf{k}} + \frac{1}{2}) \omega_{i\mathbf{k}}, \quad (2.42)$$

where the summation is over all the momentum modes and three types of excitations.

The creation and annihilation operators have the standard commutation relations

$$[a^{(-)}_{i\mathbf{k}}, a^{(+)}_{j\mathbf{p}}] = \delta_{\mathbf{kp}} \delta_{ij}. \quad (2.43)$$

Similarly, the field $\phi(x)$ can be expressed as a linear combination of the creation and annihilation operators which will be given explicitly in the next section. The particle contents of this free Hamiltonian is now clear. One has three types of excitations for each three-momentum $\mathbf{k}$. The operator $a^{(+)}_{0\mathbf{k}}$ creates an ordinary particle of mass
\(m_0\), momentum \(k\) and energy \(\omega_{0k} = \sqrt{m_0^2 + k^2}\). The operator \(a_{1k}^{(+)}\) creates a ghost particle of mass \(\mathcal{M}\), momentum \(k\) and energy \(\omega_{1k} = \sqrt{\mathcal{M}^2 + k^2}\). The operator \(a_{2k}^{(+)}\) creates an antighost particle.

### 2.3 Higher Derivative \(O(N)\) Model in the Symmetric Phase

The higher derivative field theory can be easily generalized to an \(O(N)\)-symmetric scalar field theory with a quartic coupling. In the symmetric phase it is convenient to parametrize the Lagrangian as

\[
\mathcal{L} = -\frac{1}{2} (1 + \frac{2m_0^2}{\mathcal{M}^2} \cos 2\Theta) \phi^2 \Box \phi
\]

\[
+ \left(\frac{\cos 2\Theta}{\mathcal{M}^2} + \frac{m_0^2}{2\mathcal{M}^4}\right) \phi^2 \Box \phi^2 - \frac{1}{\mathcal{M}^4} \phi^4 \Box^2 \phi^a
\]

\[-\frac{m_0^2}{2} \phi^a \phi^a - \lambda_0 (\phi^a \phi^a)^2. \tag{2.44}\]

The Hamiltonian of the theory, after indefinite metric quantization, can be expressed in terms of creation and annihilation operators, \(H = H_0 + H_{int}\), where the free part of the Hamiltonian is given by Equation (2.42). The interaction part of the Hamiltonian is the conventional one, namely \(H_{int} = \int d^3x \lambda_0 (\phi^a \phi^a)^2\), where the field \(\phi^a\) can be written as a linear combination of the creation and annihilation operators,

\[
\phi^a = \sum_p \sqrt{\frac{c_0}{2V\omega_{0p}}} \left(a_{0p}^{(-)a} e^{ip \cdot x} + a_{0p}^{(+)} e^{-ip \cdot x}\right)
\]

\[
+ \sqrt{\frac{c_1}{2V\omega_{1p}}} \left(a_{1p}^{(-)a} e^{ip \cdot x} + a_{1p}^{(+)} e^{-ip \cdot x}\right) \tag{2.45}\]
\[ + \sqrt{\frac{c_2}{2V\omega_{2p}}} (a_{2p}^{(-)a} e^{i\mathbf{p} \cdot \mathbf{x}} + a_{2p}^{(+)^a} e^{-i\mathbf{p} \cdot \mathbf{x}}), \]

where the values for \( c_i \) are given by the following list:

\[
\begin{align*}
    c_0 &= M^{-4} [(m_0^2 - M^2)(m_0^2 - \overline{M}^2)]^{-1}, \\
    c_1 &= M^{-4} [(M^2 - m_0^2)(M^2 - \overline{M}^2)]^{-1}, \\
    c_2 &= M^{-4} [(\overline{M}^2 - m_0^2)(\overline{M}^2 - M^2)]^{-1}.
\end{align*}
\]

The negative metric is seen from the adjoint relations among the creation and annihilation operators

\[
\begin{align*}
    \overline{a_{0p}^{(-)a}} \equiv \eta a_{0p}^{(-)a} \eta &= a_{0p}^{(+)^a}, \\
    \overline{a_{1p}^{(-)a}} \equiv \eta a_{1p}^{(-)a} \eta &= a_{2p}^{(+)^a}, \\
    \overline{a_{2p}^{(-)a}} \equiv \eta a_{2p}^{(-)a} \eta &= a_{1p}^{(+)^a},
\end{align*}
\]

where \( \eta \) is the metric operator satisfying \( \eta = \eta^\dagger \) and \( \eta^2 = 1 \). It is clear that the Hamiltonian itself is self-adjoint with respect to the metric \( \eta \), i.e. \( \mathcal{H} \equiv \eta H^\dagger \eta = H \).

### 2.4 Higher Derivative \( O(N) \) Model in the Broken Phase

One starts with the general higher derivative Lagrangian which has a global \( O(N) \) symmetry

\[
\mathcal{L} = \frac{1}{2} \phi^a (-\rho_1 \Box - \rho_2 \Box^2 - \rho_3 \Box^3) \phi^a + \frac{1}{2} \mu_0^2 \phi^a \phi^a - \lambda_0 (\phi^a \phi^a)^2,
\]

\((2.48)\)
where \( \Box = \partial_t^2 - \nabla^2 \) is the Minkowski space d'Alambert operator and the coefficients are parametrized as

\[
\rho_1 = 1 + \frac{m_0^2}{\mathcal{M}^2} + \frac{m_0^2}{\mathcal{M}^2}, \quad \rho_2 = \frac{1}{\mathcal{M}^2} + \frac{1}{\mathcal{M}^2} + \frac{m_0^2}{\mathcal{M}^2 \mathcal{M}^2}, \quad \rho_3 = \frac{1}{\mathcal{M}^2 \mathcal{M}^2}.
\]  

(2.49)

After the usual steps of indefinite metric quantization, the Hamiltonian has the form

\[
\mathcal{H} = i\pi_1 \phi_2^a + \frac{1}{2\rho_3} \pi_3^a \pi_3^a + \frac{1}{2} \pi_2^a (\rho_1 - 2\rho_2 \nabla^2 + 3\rho_3 \nabla^4) \pi_2^a
\]

\[
+ \frac{1}{2} \phi_1^a (-\rho_1 \nabla^2 - \rho_2 \nabla^4 - \rho_3 \nabla^6) \phi_1^a + \frac{1}{2} \phi_3^a (\rho_2 - 3\rho_3 \nabla^2) \phi_3^a + i\phi_2^a \phi_3^a
\]

\[
- \frac{1}{2} \mu_0^2 \phi_1^a \phi_1^a + \lambda_0 (\phi_1^a \phi_1^a)^2.
\]

(2.50)

The corresponding \( O(N) \) generators are given by

\[
Q^{ab} = \sum_{i,x} \phi_i^a(x) \pi_i^b(x) - \phi_i^b(x) \pi_i^a(x),
\]

(2.51)

which obviously commute with the Hamiltonian.

Next, the Fourier modes are introduced for each variable

\[
\phi_i^a(x) = \phi_i^a + \frac{1}{\sqrt{V}} \sum_{k>0} \phi_{i,k}^a e^{ik \cdot x} + \phi_{i,k}^a e^{-ik \cdot x},
\]

\[
\pi_i^a(x) = \frac{-i}{V} \frac{\partial}{\partial \phi_i^a} + \frac{-i}{\sqrt{V}} \sum_{k>0} e^{-ik \cdot x} \frac{\partial}{\partial \phi_{i,k}^a} + e^{ik \cdot x} \frac{\partial}{\partial \phi_{i,k}^a}.
\]

(2.52)

The Hamiltonian is brought into the following form:

\[
H = \frac{1}{V} (i\pi_1 \phi_{20}^a + \frac{1}{2\rho_3} \pi_{30}^a \pi_{30}^a + \frac{\rho_1}{2} \pi_{20}^a \pi_{20}^a) + V (\frac{\rho_2}{2} \phi_3^a \phi_3^a + i\phi_2^a \phi_3^a)
\]

\[
+ \sum_{k>0} i\pi_{1k}^a \pi_{2k}^a + i\pi_{1k}^a \pi_{2k}^a + \frac{1}{\rho_3} \pi_{3k}^a \pi_{3k}^a + (\rho_1 + 2\rho_2 \mathbf{k}^2 + 3\rho_3 \mathbf{k}^4) \pi_{2k}^a \pi_{2k}^a
\]
\[ + (\rho_1 k^2 + \rho_2 k^4 + \rho_3 k^6) \phi_{1k}^a \phi_{1k}^{a*} + (\rho_2 k^4 + 3\rho_3 k^2) \phi_{3k}^a \phi_{3k}^{a*} + i\phi_{2k}^a \phi_{3k}^{a*} + i\phi_{2k}^{a*} \phi_{3k}^a \]

\[ - \sum_\mathbf{x} \frac{1}{2} \mu^2_0 \phi_1^a \phi_1^a + \sum_\mathbf{x} \lambda_0 (\phi_1^a \phi_1^a)^2. \]  

(2.53)

We will single out the direction of the \( \bar{\phi}_1^a \) variable and fix it in some direction in the \( O(N) \) space. This treatment is only valid in the limit of infinite volume. Strictly speaking, in a finite volume, the symmetry is not broken. Therefore, the description of symmetry breaking in the finite volume needs more careful study. As we will show in Chapter (4), in a very large but finite volume, one can apply the adiabatic approximation (or Born-Oppenheimer Approximation) to the direction of the zeromode. We find that the direction of the zeromode rotates very slowly and decouples from the other modes in the theory. Therefore, if the volume is very large, it is legitimate to assume that the direction of the zeromode is frozen in the \( O(N) \) space.

With this in mind, we can then decompose

\[ \phi_1^a = v n^a + h(\mathbf{x}) n^a + \bar{\phi}_{1T}(\mathbf{x}), \]  

(2.54)

and similarly for the \( \phi_2 \) and \( \phi_3 \) variables. The value of \( v \) is set to \( \sqrt{\mu_0^2/4\lambda_0} \). The Hamiltonian is then written as sum of three types of terms:

\[ H = H_0 + H_{k \neq 0} + H_{\text{int}}, \]

\[ H_0 = \frac{1}{V} \left( i\pi_{10}^a \pi_{20}^a + \frac{1}{2\rho_3} \pi_{30}^a \pi_{30}^{a*} + \rho_1 \frac{\pi_{10}^a \pi_{20}^{a*}}{2} \right) + V \left( \frac{\rho_2}{2} \bar{\phi}_3^a \phi_3^a + i\bar{\phi}_2^a \phi_3^{a*} + \frac{m_0^2}{2} \sigma^2 \right), \]

\[ H_{k \neq 0} = \sum_{\mathbf{k}>0} i\pi_{1k}^a \pi_{2k}^{a*} + i\pi_{1k}^{a*} \pi_{2k}^a + \frac{1}{\rho_3} \pi_{3k}^a \pi_{3k}^{a*} + (\rho_1 + 2\rho_2 k^2 + 3\rho_3 k^4) \pi_{2k}^a \pi_{2k}^{a*} \]

\[ + (\rho_1 k^2 + \rho_2 k^4 + \rho_3 k^6 + m_0^2) \phi_{1kL}^a \phi_{1kL}^{a*} + (\rho_1 k^2 + \rho_2 k^4 + \rho_3 k^6) \phi_{1kT}^a \phi_{1kT}^{a*} \]

\[ \phi_1^a = v n^a + h(\mathbf{x}) n^a + \bar{\phi}_{1T}(\mathbf{x}), \]
\[ H_{\text{int}} = \sum_k 4\lambda_0 v h (h^2 + \tilde{\phi}_1^a \tilde{\phi}_1^a) + \lambda_0 (h^2 + \tilde{\phi}_1^a \tilde{\phi}_1^a)^2, \]  

(2.55)

where \( m_0^2 = 2\mu^2 \). We will examine each piece separately.

The \( k \neq 0 \) piece can be diagonalized the same way as in section (2.3). The interaction piece is also expressed as the creation and annihilation operators through the field variables. The \( H_0 \) piece is the only one that is new in the broken phase. For convenience we use the rescaled variables given by

\[ p_1^a = (\rho_1 V)^{-1/2} n_{10}^a, \quad p_2^a = \sqrt{\frac{\rho_1}{V}} n_{20}^a, \quad p_3^a = (\rho_3 V)^{-1/2} n_{30}^a, \]

\[ q_1^a = (\rho_1 V)^{1/2} \tilde{\phi}_1^a, \quad q_2^a = \sqrt{\frac{V}{\rho_1}} \tilde{\phi}_2^a, \quad q_3^a = (\rho_3 V)^{1/2} \tilde{\phi}_3^a, \]  

(2.56)

and express the radial variables \( q_1^a \) as

\[ q_1^a = \sqrt{\rho_1 V} (\nu + \sigma) n^a = \rho n^a. \]  

(2.57)

The derivatives for the \( q_1^a \) are now substituted by

\[ \frac{\partial}{\partial q_1^a} = n^a \frac{\partial}{\partial \rho} \]  

(2.58)

where the index \( a \) runs from 1 to \( N \). We have assumed that the volume is practically infinite and the direction \( n^a \) is really a constant unit vector in \( O(N) \) space. As we will see in Chapter (4), this is only approximately true in a finite volume. Use the following identity

\[ ip_1^a p_2^a = ip_{2L} p_{1\rho}, \]  

(2.59)
$H_0$ is further decomposed into two parts

$$H_0 = H_{0L} + H_{0T},$$

$$H_{0L} = ip_{2L}p_y + \frac{1}{2} p_{2L}^2 + \frac{1}{2} p_{3L}^2 + \frac{\rho_2}{2\rho_3} q_{3L}^2 + i\sqrt{\frac{\rho_1}{\rho_3}} q_{2L} q_{3L} + \frac{m_0^2}{2\rho_1} y^2,$$

$$H_{0T} = \frac{1}{2} p_{2T}^2 + \frac{1}{2} p_{3T}^2 + \frac{\rho_2}{2\rho_3} q_{3T}^2 + i\sqrt{\frac{\rho_1}{\rho_3}} q_{2T} q_{3T}.$$

The longitudinal part has the same form as the simple oscillator and can be easily diagonalized. The transverse part $H_{0T}$ can also be diagonalized with the transformation

$$q_T = Aq_T, \quad AA^T = A^T A = 1,$$

where $A$ is a two by two matrix

$$A = \begin{pmatrix} -1/(1-e^{-4i\theta_g})^{1/2} & 1/(1-e^{4i\theta_g})^{1/2} \\ -i\sqrt{(1-e^{-4i\theta_g})^{1/2}} & i\sqrt{(1-e^{4i\theta_g})^{1/2}} \end{pmatrix}.$$  \hspace{1cm} (2.62)

The angle $\theta_g$ is the complex phase of the Goldstone ghost mass parameter $\mathcal{M}_g = |\mathcal{M}_g|e^{i\theta_g}$, which is given by

$$\mathcal{M}_g^2 = \frac{m_0^2 + \mathcal{M}_g^2}{2} + i\mathcal{M}_g \sqrt{\rho_1 - \frac{1}{4} \left( \frac{m_0^2}{\mathcal{M}_g} + \frac{\mathcal{M}_g}{\mathcal{M}} + \frac{\mathcal{M}}{\mathcal{M}_g} \right)^2}.$$  \hspace{1cm} (2.63)

The transverse part of the Hamiltonian is then diagonalized to

$$H_{0T} = \sum_{a \neq 0} q_{aT}^{(+)} a_{aT}^{(-)} \omega_{aT},$$

where the summation of $a$ is from 1 to $N$ and the energy gap is $\omega_{10T} = \mathcal{M}_g$ and...
\( \omega_{0T} = \overline{M}_g \). In terms of these operators we can write out the explicit form of \( p_{2T}^a \):

\[
p_{2T}^a = \sum_{i \neq 0} \sqrt{\frac{\omega_{0T}}{2}} \epsilon_i, (a_{i0T}^{(-)} a_{i0T}^{(+)a})
\]

(2.65)

where the polarization factor \( \epsilon_i \) is given by \( \epsilon_1 = \epsilon_2^* = i/(1 - e^{-4i\theta_g})^{1/2} \).

To summarize, in the broken phase we would have the following Hamiltonian:

\[
H = H_0 + H_{\text{int}},
\]

\[
H_0 = \sum_{i,k,\lambda} a_{i k \lambda}^{(+)} a_{i k \lambda}^{(-)} \omega_{i k \lambda},
\]

\[
H_{\text{int}} = \sum_{x} 4 \lambda_0 v h (h^2 + \tilde{\phi}_1^a \tilde{\phi}_1^a) + \lambda_0 (h^2 + \tilde{\phi}_1^a \tilde{\phi}_1^a)^2.
\]

(2.66)

The index \( \lambda \) takes the value \( L \) and \( T \) respectively. All the operators can be expressed in terms of the creation and annihilation operators as

\[
h(x) = \sum_{ik} \frac{c_{iL}}{\sqrt{2 \omega_{ijkL}}} \left( n_i^a a_{i k L}^{(-)} e^{i k \cdot x} + n_i^a a_{i k L}^{(+)a} e^{-i k \cdot x} \right),
\]

\[
\tilde{\phi}_1^a(x) = \sum_{ik \neq 0} \frac{c_{i T}}{\sqrt{2 \omega_{ikT}}} \left( a_{i k T}^{(-)} e^{i k \cdot x} + a_{i k T}^{(+)a} e^{-i k \cdot x} \right),
\]

(2.67)

\[
\rho = \sqrt{\rho_1 V (v + \sigma)} = \sqrt{\rho_1 V} \left( v + \sum_i \frac{c_{i L}}{\sqrt{2 \omega_{i0L}}} (a_{i0L}^{(-)} + a_{i0L}^{(+)a}) \right),
\]

where the form factors \( c_{i \lambda} \) are given by the following table:

\[
c_{0L} = \sqrt{\frac{M^2 \overline{M}_g^2}{(m_0^2 - M^2)(m_0^2 - \overline{M}_g^2)}}, \quad c_{1L} = c_{2L}^* = \sqrt{\frac{M^2 \overline{M}_g^2}{(M^2 - m_0^2)(M^2 - \overline{M}_g^2)}},
\]

\[
c_{0T} = 1, \quad c_{1T} = c_{2T}^* = \sqrt{\frac{\overline{M}_g^2}{(M_0^2 - \overline{M}_g^2)}},
\]

(2.68)
The creation and annihilation operators enjoy the following commutation relations

\[ [a^{(-)a}_{ik\lambda}, a^{(+)b}_{jp\lambda'}] = \delta_{ij} \delta_{kp} \delta_{\lambda\lambda'} P_{\lambda}. \]  

(2.69)
References

[1] M. Ostrogradski, Mem. Ac. St. Petersbourg 4 (1850) 385.

[2] B. Podolski, Phys. Rev. 62 (1942) 68; B. Podolski and P. Schwed, Rev. Mod. Phys. 20 (1948) 40.

[3] A. Pais and G. E. Uhlenbeck, Phys. Rev. 79 (1950) 145

[4] T. D. Lee and G. C. Wick, Nucl. Phys. B 9 (1969) 209; Phys. Rev. D 2 (1970) 1033.

[5] K. Jansen, J. Kuti, C. Liu Phys. Lett. B 309 (1993) 119.

[6] D. G. Boulware and D. J. Gross, Nucl. Phys. B233 (1983) 1.

[7] W. Pauli, Rev. Mod. Phys. 15 (1943) 175.

[8] J. Z. Simon, Phys. Rev. D41 (1990) 3720.

[9] A. A. Slavnov, Nucl. Phys. B31 (1971) 301.

[10] S. W. Hawking, Quantum field theory and quantum statistics, eds. I. A. Batalin et al. (1987) p. 129.
Chapter 3

Unitarity and Large $N$ Expansion

3.1 Lippmann-Schwinger Equation And Unitarity

In this section, we will try to answer one of the most important questions about higher derivative theories, namely, the unitarity problem [1, 2, 3, 4, 5]. In the first part of the discussion, we will set up the general formalism of scattering matrix in the higher derivative theory and argue that the $S$-matrix defined within the physical subspace can be made unitary. In the second part, we will present a concrete example of the unitary scattering amplitude in the large $N$ limit of the $O(N)$ model which involves the ghost states as intermediate states.

3.1.1 General Formalism and Unitarity

Let us imagine that our Hilbert space is built up by all the states generated from the vacuum by successive operations of creation operators as described in Chapter (2). Some states will have negative norm and complex energy components. We assume that all states available to build the initial state contain only real energy components of the free Hamiltonian in all Lorentz frames [2]. We will call these states “normal states” or “physical states”. Denote the eigenstate of the free
Hamiltonian by \( |\phi_\alpha\rangle \) such that

\[
H_0 |\phi_\alpha\rangle = E_\alpha |\phi_\alpha\rangle, \tag{3.1}
\]

\[E_\alpha \in \mathbb{R}.
\]

Then one can construct two states, denoted as \( |\psi_\alpha^{(+)}\rangle \) and \( |\psi_\alpha^{(-)}\rangle \), from the Lippmann-Schwinger equation

\[
|\psi_\alpha^{(\pm)}\rangle = |\phi_\alpha\rangle + \frac{1}{E_\alpha - H_0 \pm i\epsilon} V |\psi_\alpha^{(\pm)}\rangle, \tag{3.2}
\]

\[
|\psi_\alpha^{(\pm)}\rangle = |\phi_\alpha\rangle + \frac{1}{E_\alpha - H \pm i\epsilon} V |\phi_\alpha\rangle.
\]

It is then easy to show that the states \( |\psi_\alpha^{(\pm)}\rangle \) are eigenstates of the full Hamiltonian with corresponding energy \( E_\alpha \). If we now form wavepackets from these states, one can see that they correspond to incoming and outgoing waves in the past or future. Therefore, they give us a good description of the scattering process. We can rewrite the above equation as

\[
|\psi_\alpha^{(\pm)}\rangle = \pm i\epsilon \frac{1}{E_\alpha - H \pm i\epsilon} |\phi_\alpha\rangle. \tag{3.3}
\]

In this form, it is clear that only energy conserving components of \( |\phi_\alpha\rangle \) survive the scattering since, if the components are of different energy, they will make the operator \((E_\alpha - H \pm i\epsilon)^{-1}\) nonsingular in the \( \epsilon \) goes to zero limit, hence are killed by the \( \epsilon \) in front. The \( S \)-matrix between any two normal states \( \alpha \) and \( \beta \) is then defined to be

\[
S_{\beta\alpha} \equiv \langle \psi_\beta^{(-)} | \eta | \psi_\alpha^{(+)\rangle} \tag{3.4}
\]

\[
= \langle \phi_\beta | \eta \frac{i\epsilon}{E_\beta - H} \frac{i\epsilon}{E_\alpha - H} \frac{i\epsilon}{|\phi_\alpha\rangle}.
\]
Using the perturbative expansion of the Green's function one can show that the
$S$-matrix element defined above is related to the so called $R$-matrix (or $T$-matrix)
element by

\[ S_{\beta \alpha}(E_{\alpha}) = \delta_{\beta \alpha} - 2\pi i \delta(E_{\alpha} - E_{\beta}) R_{\beta \alpha}(E_{\alpha}), \]

\[ R_{\beta \alpha}(E_{\alpha}) = \langle \phi_{\beta} | R(E_{\alpha}) | \phi_{\alpha} \rangle, \]

\[ R(E) = V + V \frac{1}{E - H_{0} + i\epsilon} R(E), \]  
\[ (3.5) \]

\[ R(E) = V + V \frac{1}{E - H_{0} + i\epsilon} V + \cdots, \]

\[ R(E) = V + V \frac{1}{E - H + i\epsilon} V. \]

To show unitarity, we write the Lippmann-Schwinger equation in a special way

\[ |\psi_{\alpha}^{(\pm)}\rangle = \Omega^{(\pm)}(E_{\alpha}) |\phi_{\alpha}\rangle, \]

\[ (3.6) \]

\[ \Omega^{(\pm)}(E_{\alpha}) = 1 + \frac{1}{E_{\alpha} - H \pm i\epsilon} V \frac{\pm i\epsilon}{E_{\alpha} - H_{0} \pm i\epsilon}, \]

where $\Omega^{(+)}(E_{\alpha})$ and $\Omega^{(-)}(E_{\alpha})$ are called wave operators. Using the adjointness of
the Hamiltonian we see that

\[ |\phi_{\alpha}\rangle = \eta \Omega^{(\pm)}(E_{\alpha})^{\dag} \eta |\psi_{\alpha}^{(\pm)}\rangle. \]

\[ (3.7) \]

From these two relations we can see that

\[ \eta \Omega^{(\pm)}(E_{\alpha})^{\dag} \eta \Omega^{(\pm)}(E_{\alpha}) = 1 + P_{c}, \]  
\[ (3.8) \]
where $P_c$ is the complex energy projector for the free Hamiltonian. Let us now consider the sum

$$\sum_{\alpha, E_{\alpha} \in \mathbb{R}} S_{\beta\alpha} S_{\gamma\alpha}^{*} = \sum_{\alpha} \langle \psi^{(-)}_{\beta} | \eta | \psi^{(+)}_{\alpha} \rangle \langle \psi^{(+)}_{\alpha} | \eta | \psi^{(-)}_{\gamma} \rangle$$

$$= \langle \psi^{(-)}_{\beta} | \eta | \psi^{(-)}_{\gamma} \rangle$$

$$= \langle \phi_{\beta} | \Omega^{(-)}(E_{\beta})^{\dagger} \eta \Omega^{(-)}(E_{\beta}) | \phi_{\gamma} \rangle$$

$$= \langle \phi_{\beta} | \eta | \phi_{\gamma} \rangle = \delta_{\beta\gamma}, \quad (3.9)$$

where, in the second step, we have inserted the complete set of the full Hamiltonian. This establishes the unitarity of the $S$-matrix. The above proof looks very formal.

To clearly understand the role of the ghost states in the theory let us calculate some scattering processes in the higher derivative $O(N)$ model.

### 3.1.2 Large-$N$ Scattering Amplitude of $O(N)$ Model

The basic formula is the perturbation expansion of the $S$-matrix given by Equation (3.5). We will consider the large-$N$ limit of the geometric resummation of the $s$-channel bubble diagram. We will show how the modified Feynman Rules arise naturally from this calculation.

First, we calculate the $R$-matrix elements to second order in bare perturbation theory of the higher derivative $O(N)$ theory in the broken phase. The final large $N$ scattering amplitude can then be formed from the geometric resummation of the bubbles and the large $N$ Higgs propagator. The calculation in the symmetric phase
is quite similar. We will parametrize the $R$-matrix elements as

$$R_{\alpha\beta} = -(2\pi)^3 \delta^3(\sum p) \prod_{\text{ext}} \sqrt{\frac{c}{2\omega V}} M_{\alpha\beta}, \quad (3.10)$$

where the amplitude $M_{\alpha\beta}$ is the Feynman amplitude. The lowest order is trivial namely

$$M^{(1)}_{\alpha\beta} = -8\lambda_0. \quad (3.11)$$

To the second order, we have to consider the intermediate states contributions and, in the large-$N$ limit, this reduces to only $s$-channel scattering. This leads us to the study of the following one loop contribution,

$$M^{(2)}_{\alpha\beta} = 96N^2\lambda_0^2 \int \frac{d^3q}{(2\pi)^3} \left( \frac{c_ic_j}{2\omega_i q^2 \omega_j p-q} \right) \frac{2(\omega_i q + \omega_j p-q)}{E^2 - (\omega_i q + \omega_j p-q)^2 + i\epsilon}. \quad (3.12)$$

in which two types of intermediate states are included, one has energy $\omega_i q + \omega_j p-q$, the other has energy $2E + \omega_i q + \omega_j p-q$. This form can be brought into the usual loop integral form by using the identity

$$\int_c dq_0 \frac{1}{2\pi} \frac{1}{(q_0 - E)^2 - \omega_1^2 q_0^2 - \omega_2^2} = -i \frac{2(\omega_1 + \omega_2)}{2\omega_1 \omega_2 E^2 - (\omega_1 + \omega_2)^2 + i\epsilon}, \quad (3.13)$$

where the complex contour is a contour that separates $E - \omega_1$ and $-\omega_2$ from $E + \omega_1$ and $\omega_2$ as shown in Figure (3.1). However, this type of contour could have some pinching problem [2, 3]. The problem only occurs for the ghost and antighost pair contribution in the above equation, i.e. $\omega_1 = \omega_2^*$. In order to see how the potential pinching problem occurs, we have shown the movement of the poles in the complex $q_0$ plane as the center of mass energy increases in Figure (3.1) The appropriate contour before the pinching is also shown. It is easy to see that if the center of mass energy $E$ is less than the so called ghost antighost threshold $\omega_1 + \omega_2 = 2Re\omega_1$, there is no pinching and the contour is well defined. As the center of mass energy increases,
Figure 3.1: The complex contour of the integration variable $q_0$. The triangles are the poles from one of the ghost antighost contributions. The squares are the poles when the roles of $\omega_1$ and $\omega_2$ are interchanged. As the center of mass energy $E$ increases, the movement of the poles are also shown by the arrows. Pinching occurs when $E > (\omega_1 + \omega_2)$.

four of the eight poles move to the right and two of them pinch with $\omega_1$ and $\omega_2$. One then has to specify how to deform the contour in the case of pinching. This type of contour deformation in the presence of possible pinching was also discussed before by Cutkosky et al. [3]. They started directly from the integral representation and tried to define a contour when the ghost and antighost masses are not exactly complex conjugate of each other, namely $M_1 - M_2^* = i\Delta$, where $\Delta$ is some small parameter. Then, for every nonvanishing $\Delta$, they were able to find a suitable contour. The final result is defined to be the limit where $\Delta \to 0$. The corresponding contour is shown in Figure (3.2). This prescription has a disadvantage that it is not justified with any theoretical consideration. In fact, the Cutkosky prescription is only one of the many ways to analyticly continue the integral (3.13). To specify the “right”
Figure 3.2: The complex contour of the integration variable \( q_0 \) as discussed by Cutkosky et al. The pinching is avoided by splitting the ghost and antighost masses by a small imaginary amount.

analytic continuation, one would need some input from the Hamiltonian description of the theory. We have started from the Hamiltonian picture of the theory, so the Hamiltonian should tell us how to define our contour. Note that pinching only occurs when the \( i\epsilon \) prescription is not applied to the integral. With the \( i\epsilon \), however, the pinching is avoided for real value of \( s \) and we can always find a suitable contour. This contour is shown in Figure (3.3). It is clear that our contour differs from the one discussed by Cutkosky et al. and therefore, our final result is different from theirs. Now the Feynman amplitude can be expressed as

\[
M^{(2)}_{\alpha\beta} = -i96N\lambda_0^2 \sum_{i,j} \int_{C_{ij}} \frac{d^4 q}{(2\pi)^4} \frac{c_j}{q_0^2 - \omega^2_{j,q} + i\epsilon} \frac{c_i}{(q_0 - E)^2 - \omega^2_{i,p-a} + i\epsilon}.
\] (3.14)

This amplitude represents the Feynman diagram as shown in Figure (3.4). We can shift the integration variable \( q_0 \) and after a Wick rotation we can perform the \( q \)
Figure 3.3: Our complex contour of the integration variable \( q_0 \) in the presence of possible pinching. The pinching is avoided by using the \( +i\epsilon \) prescription which is derived naturally from the Lippmann-Schwinger formalism of the Hamiltonian.

The integral itself is finite due to the modification of the propagator at large momentum and we are left with an integral with Feynman parameter only

\[
\mathcal{M}^{(2)}_{\alpha\beta} = 96 N \lambda^2_0 B(s),
\]

\[
B(s) = \frac{-1}{16\pi^2} \sum_{i,j} c_i c_j \int_0^1 dx \log[x m_i^2 + (1-x)m_j^2 - x(1-x)s].
\]

(3.15)

It is very interesting to study the imaginary part of the bubble integral. The imaginary part comes only from the angular part of the argument in the logarithm. The function being quadratic in \( x \) has two roots in the complex \( x \) plane which are given by

\[
F(s) \equiv x m_1^2 + (1-x)m_2^2 - sx(1-x) = s(x - x_1)(x - x_2),
\]
Figure 3.4: The $s$-channel one loop amplitude of Goldstone Goldstone scattering. The solid lines represent incoming and outgoing Goldstone particles. The dashed line can be Goldstone particle, Goldstone ghost or antighost particle.

\[ x_{1,2} = \frac{1}{2s}(s - m_1^2 + m_2^2) \pm \sqrt{(s - (m_1 + m_2)^2)(s - (m_1 - m_2)^2)}, \quad (3.16) \]

where $m_1$ and $m_2$ can take values of three different masses in the theory. The most important combination is when both are Goldstone particles. Then, for $s < 0$, we have two conjugate roots whose real part is exactly $1/2$, therefore, just by symmetry, there is no imaginary part contribution from this term. This corresponds to the case that the center of mass energy is less than the threshold. Due to the massless Goldstone, the lowest threshold is at zero energy. However, when $s > 0$ two roots are real and the imaginary part develops, we have

\[ \Im B(s + i\epsilon) = \frac{1}{16\pi}. \quad (3.17) \]

In fact one can show, just from the symmetric form of the integral, that this is the only imaginary part contribution to the diagram! For example the imaginary part from the mass pair $\mathcal{M}$ and $\mathcal{M}$ exactly cancels the imaginary part from the mass pair $\mathcal{M}$ and $\mathcal{M}$ and so on. In the large-$N$ limit the scattering amplitude is obtained by summing the geometric chain of the bubbles and the tree contribution from the
intermediate Higgs state

\[- \frac{N}{32\pi} A_{00}^{-1}(s) = \frac{v^2}{s + s^3/M^4} + \frac{1}{8\lambda_0} + \frac{N}{2} B(s). \] (3.18)

Taking the imaginary part of this equation, we get the Optical Theorem in the large-$N$ limit

\[ \Im A_{00}(s) = |A_{00}(s)|^2. \] (3.19)

The bubble integral can be exactly worked out. It is a function with rather complicated analytic structure. The detailed discussion is listed in the appendix.

The scattering amplitude is obtained by taking \( s = |s| + i\epsilon \) on the physical sheet. It is interesting to study the Goldstone-Goldstone scattering cross section in the large-$N$ limit. In Figure (3.5) we plotted the cross section as a function of \( \sqrt{s} \) in Goldstone ghost mass unit. Here the Goldstone ghost pair has a complex phase of \( \pi/4 \) and the peak corresponds to the Higgs pole on the second sheet. It is amazing that the ghost pair is so well-hidden in the tail of the cross section that it would be very difficult for experimentalists to determine that there is a ghost pair hidden somewhere. Also plotted in Figure (3.5) is the scattering phase shift as a function of center of mass energy. We see that the phase shift starts out increasing with \( \sqrt{s} \), and at the Higgs pole it has a sharp rise. If the Higgs particle were infinitely narrow then the rise would be exactly \( \pi \). Due to the finiteness of its width and the Goldstone background, the cross section differs from the description of Breit-Wigner shape.

What is “unusual” about this theory is that the phase shift decreases as the energy gets through the real part of the ghost mass. This is an indication of possible acausal behavior in the scattering, because the sign of \( d\delta(s)/ds \) determines the relative phase of the scattered wave to the incident wave. Although for the scattering by a repulsive potential in the usual theory, this quantity can also be negative, it would become
Figure 3.5: The Goldstone Goldstone scattering cross section and phase shift is plotted against the center of mass energy in large-$N$ expansion for the Pauli-Villars higher derivative $O(N)$ theory. The input vev value is $v = 0.07$ in $M$ unit. The peak corresponds to the Higgs resonance, which is at $m_H = 0.28$ in $M$ unit. The scattering cross section is completely smooth across the so-called ghost pole locations.

acausal if this quantity becomes too large, that is, a sharp drop of $\delta(s)$ with respect to $s$. In the ordinary theory, this can never happen. In the higher derivative theory with the ghost pair, it could happen if the ghost pair is sufficiently close to the real axis. It had been argued long ago by T. D. Lee [2] that, even in this case, such acausal behavior would only occur at microscopic scale typical of the Compton wave length of the ghost, and it will not lead to macroscopic disasters. In fact, this violation of microscopic causality is barely visible experimentally.
3.2 Large $N$ Expansion of the Higher Derivative $O(N)$ Model

The higher derivative $O(N)$ model can be studied in the large $N$ limit. Many aspects of the theory can be illustrated in the large $N$ expansion [6, 7]. The general formalism for the large $N$ expansion has been previously studied [9, 10]. Let us briefly review the main ideas and focus on its application to the higher derivative $O(N)$ model, and also emphasize the comparison of the higher derivative $O(N)$ model with the conventional $O(N)$ model within the large $N$ approximation. The Hamiltonian picture that originates from the quantization was discussed in the last section, so we will only consider the Euclidean version of the large $N$ approximation here.

3.2.1 General Formalism

Consider the partition function of the theory as expressed by the following Euclidean path integral

$$Z = \int \mathcal{D}\phi e^{-S[\phi]},$$

$$S[\phi] = \int d^4x \frac{1}{2} \phi^a g(-\partial^2) \phi^a + \frac{\mu_0^2}{2} \phi^a \phi^a + \frac{\lambda_0}{N} (\phi^a \phi^a)^2,$$  \hspace{1cm} (3.20)

where the field $\phi^a(x)$ is an $O(N)$ field and the function $g(-\partial^2)$ is a polynomial function of the operator $(-\partial^2)$ of the form

$$g(-\partial^2) = (-\partial^2) + c_4(-\partial^4) + c_6(-\partial^6) + \cdots.$$  \hspace{1cm} (3.21)

For example, our choice of the Pauli-Villars theory corresponds to the form of $g(p^2) = p^2 + (1/M^4)p^6$. To perform the large $N$ expansion, it is convenient to introduce the
auxiliary fields $\chi$ such that the path integral is rewritten in the following form

$$Z = \int D\phi D\chi \exp(-\int d^4x \frac{1}{2} \phi^a (g(-\partial^2) + \mu_0^2 + i\chi) \phi^a + \frac{N\chi^2}{4\lambda_0}). \quad (3.22)$$

The effective potential can then be worked out in a standard fashion

$$U(\bar{\phi}) = \frac{1}{2} \bar{\phi}^2 \bar{\chi} - \frac{1}{16\lambda_0} \bar{\chi}^2 + \frac{\mu_0^2}{8\lambda_0} \bar{\chi} + \frac{N}{2} \int \frac{d^4k}{(2\pi)^4} \log(g(k^2) + \bar{\chi}), \quad (3.23)$$

where the variable $\bar{\chi}$ is a function of $\bar{\phi}$ determined from the gap equation

$$\bar{\chi} = \mu_0^2 + 4\lambda_0 \bar{\phi}^2 + 4\lambda_0 N \int \frac{d^4k}{(2\pi)^4} \frac{1}{g(k^2) + \bar{\chi}}. \quad (3.24)$$

The vacuum can be found from the derivative of the above effective potential. Due to the gap equation, the derivative has the following form

$$U'(\bar{\phi}) = \bar{\phi} \bar{\chi}. \quad (3.25)$$

Therefore there could be two phases of the theory. One with $\bar{\phi} = 0, \bar{\chi} \neq 0$, which is the symmetric phase; the other one has $\bar{\phi} \neq 0, \bar{\chi} = 0$, which is the broken phase. In the broken phase, the vacuum expectation value is obtained via

$$0 = \mu_0^2 + 4\lambda_0 v^2 + 4\lambda_0 N \int \frac{d^4k}{(2\pi)^4} \frac{1}{g(k^2)}. \quad (3.26)$$

Note that unlike the conventional theory, the integral in the above equation is finite as long as we have take the highest momentum power in the propagator to be greater or equal to 6. The critical phase transition line is obtained by setting $v$ to zero in the above equation, i.e.

$$0 = \mu_0^2 + 4\lambda_0 N \int \frac{d^4k}{(2\pi)^4} \frac{1}{g(k^2)}. \quad (3.27)$$

As we will see in Chapter (4), the large $N$ prediction of the critical line is in very good agreement with the simulation.
We can work out the propagator of the fields in the large $N$ approximation. If we are in the symmetric phase, the leading order correction to the propagator is just from the mass renormalization. Therefore, we have

$$< \phi^a(p) \phi^b(p) > = \frac{\delta^{ab}}{p^2 + m^2},$$

$$m^2 = \mu_0^2 + 4\lambda_0 N \int \frac{d^4k}{(2\pi)^4} \frac{1}{g(k^2) + m^2}, \quad (3.28)$$

In the broken phase, the Goldstone propagator remains unchanged to the leading order but the longitudinal Higgs propagator is modified by the bubble summation of the Goldstone intermediate states. Thus, we have

$$\Gamma_{\sigma\sigma}(p^2) = g(p^2) + \frac{8\lambda_0 v^2}{1 + 4\lambda_0 NB(p^2)},$$

$$B(p^2) = \int \frac{d^4k}{(2\pi)^4} \frac{1}{g((p-k)^2)g(k^2)} \quad (3.29)$$

The scattering amplitude can be worked out in both the symmetric and broken phase. In the symmetric phase,

$$-\frac{N}{32\pi} A^{-1}_{00}(p^2) = \frac{1}{24\lambda_0} + \frac{N + 8}{6} I(p^2),$$

$$I(p^2) = \int \frac{d^4k}{(2\pi)^4} \frac{1}{g((k-p)^2) + m^2)(g(k^2) + m^2)}, \quad (3.30)$$

where $m^2$ is related to the bare mass parameter $\mu_0^2$ according to Equation (3.28). If we define the scattering amplitude at $p^2 = 0$ to be $-3N/4\pi\lambda_R$, we can express the above equation in terms of the renormalized coupling constant $\lambda_R$

$$-\frac{N}{32\pi} A^{-1}_{00}(p^2) = \frac{1}{24\lambda_R} + \frac{N + 8}{6}[I(p^2) - I(0)], \quad (3.31)$$
In the broken phase, we have

$$-\frac{N}{32\pi}A_{00}^{-1}(p^2) = \frac{1}{8\lambda_0} + \frac{N}{2} \int \frac{d^4k}{(2\pi)^4} \frac{1}{g((k-p)^2)g(k^2)} + \frac{v^2}{g(p^2)}. \quad (3.32)$$

Note that although we are dealing with the Euclidean scattering amplitude here in large $N$, it should be understood as the amplitude arising from the Hamiltonian formalism described in the previous section. As long as the correct complex contour integration is implemented, and the analytic properties of these amplitudes are understood, the Euclidean amplitude will also give us the correct physical picture.

We can also modify the above formalism to the theory on the lattice in a finite volume. All we have to do is to change the integral into finite lattice summations.

Let us now show some examples of the application of the large $N$ results and see what we can learn from it.

### 3.2.2 Renormalized Coupling Constant in the Symmetric Phase

In the first example, we compare the higher derivative $O(N)$ model on the lattice and the conventional $O(N)$ model on the lattice in the symmetric phase. As described in Equation (3.31), the renormalized coupling constant $\lambda_R$ can be defined as

$$\lambda_R = \frac{\lambda_0}{1 + 4\lambda_0(N + 8)I(0)},$$

$$I(0) = \frac{1}{V} \sum_k \frac{1}{(g(k^2) + m^2)^2}, \quad (3.33)$$

where everything is measured in lattice unit. In this formula, the factor $(N + 8)$ is the exact group theory factor. However, in the naive large $N$ approximation, we should use $N$ instead of $(N + 8)$. When we apply this to the $O(4)$ model, this makes
a factor of 3 difference. We therefore have to conclude that the leading order large $N$ results are ambiguous when applied to $N = 4$. As we will see in the next example, similar situation occurs for the broken phase. We can calculate this renormalized coupling constant at the same correlation length $\xi \equiv 1/m$ in the conventional $O(N)$ model and in the Pauli-Villars theory, with some fixed value of $M$, for every value of the bare coupling constant $\lambda_0$. The magnitude of this quantity reflects the strength

![Graph](image)

**Figure 3.6:** The comparison of the large $N$ renormalized coupling constant in the symmetric phase is shown for three cases: continuum Pauli-Villars, lattice Pauli-Villars and the conventional $O(N)$ model. For this choice of the correlation length, the lattice effects are small and the Pauli-Villars theory shows much stronger interaction when compared with the conventional $O(N)$ model. We have modified the naive large $N$ formula so that the right group theory factor is substituted, i.e. $N + 8 = 12$.

of the interaction in the symmetric phase. In Figure (3.6), the comparison between the two theories is shown for $m = 0.3, M = 1.0$ for every given $\lambda_0$. The lattice
summation is calculated on a $32^4$ lattice with the naive lattice discretization of the Laplacian. The continuum Pauli-Villars result is also shown in the figure. For this choice of the correlation length, the lattice effects are rather small in both theories. It is clear that the Pauli-Villars theory has stronger interaction, about a factor of 4, for the same correlation length when compared with the conventional $O(N)$ model. As mentioned above, the large $N$ expansion has its own ambiguities, so we do not anticipate this large $N$ result to give us a precise quantitative description of the theory. However, we do expect that the increase of the coupling constant in the Pauli-Villars theory relative to the conventional theory should also be present in the full theory. Similar results in the broken phase also support this picture, as we will see in the next subsection.

### 3.2.3 Higgs Mass and Width for Conventional $O(N)$ Model

Now, we will examine the situation in the broken phase of the theory. We will first briefly review the large $N$ result for the conventional $O(N)$ model with a hypercubic lattice regulator [9, 10] in the broken phase. The large $N$ Goldstone propagator will remain the free propagator in the leading order of $1/N$ expansion, but the large $N$ Higgs propagator will be

$$\Gamma_{\sigma\sigma}(p^2) = \hat{p}^2 + \frac{8\lambda_0 v^2}{1 + 4\lambda_0 N B(p^2)}.$$  

$$B(p^2) = \int \frac{d^4k}{(2\pi)^4} \frac{1}{(p-k)^2 k^2}. \quad (3.34)$$

In general, the lattice bubble is a very complicated function of $p$. However in the limit of small $p^2$, which is the regime of physical interests, it has been worked out
and has the following asymptotic expression [8]

\[ B(p^2) = \frac{1}{16\pi^2}(-\log(p^2) + c_{\text{lat}} + O(p^2)), \]

where the constant \( c_{\text{lat}} = 5.79200957 \) for the hypercubic lattice. We can now use this relation to find the complex pole to the Higgs propagator. Since the higher order terms are neglected in the bubble, it is sufficient to keep only the leading term in the lattice momentum. Setting \((-p^2) = s = (m_H - i\Gamma_H/2)^2 = r^2e^{-2i\theta}\), we have (taking the second Riemann sheet value for the logarithm)

\[ r = \sqrt{\frac{32\pi^2v^2}{N} \frac{\sin 2\theta}{\pi + 2\theta}}, \]

\[ \cos 2\theta = \frac{\sin 2\theta}{\pi + 2\theta} \left( \frac{4\pi^2}{\lambda_0N} + c_{\text{lat}} - \log \frac{32\pi^2v^2}{N} - \log \frac{\sin 2\theta}{\pi + 2\theta} \right). \]

The phase \( \theta \) is first determined from the second equation and then substituted into the first one to get the real and imaginary part of the Higgs pole. The result is summarized in Figure (3.7). For the Higgs correlation length of about 2, the ratio \( m_H/v \) is only about 3. The correlation length 2 is chosen because if the Higgs is too heavy in lattice units, the lattice effects would become significant and the theory would no longer describe continuum physics [8].

Another feature that we can study is the width of the Higgs particle. There has been quite a lot of confusion even with the conventional \( O(N) \) model. The large \( N \) width of the \( O(N) \) model was first carefully studied by Einhorn using a sharp momentum cutoff [10]. He found that the large \( N \) formula, if \( N = 4 \) is substituted in, gives too large a width (40 percent larger) when compared with the perturbation theory of the \( O(N = 4) \) model. Therefore, the large \( N \) results seem to indicate that the theory is more strongly interacting than the perturbative predictions. Some authors interpret this finding as genuine nonperturbative effects of the model [9].
Figure 3.7: The large $N$ result of the Higgs mass over vev ratio $m_H/v$ as a function of the bare coupling constant for the conventional $O(N)$ model with a hypercubic lattice regulator. Four curves correspond to different $v$ values (in lattice units) as indicated. $N$ has been set to 4 in the calculation.

However, we do not think this is true for the following two reasons. First of all, the large $N$ result of the width does not agree with perturbation theory, even for very weak couplings. In this regime, the next to leading term of the width has been calculated in perturbation theory. The correction is very small, typically of the order of one percent. Therefore, it is unlikely that even higher order terms will change this perturbative result significantly. Secondly, the perturbative result has been proven to be correct by extensive nonperturbative Monte Carlo simulation studies. No mysterious nonperturbative effects as predicted by large $N$ have been found.

We believe this discrepancy is because of the ambiguity within the large $N$
framework. The large $N$ result can only be accurate to about 20 to 30 percent because of the large subleading $1/N$ terms at $N = 4$. After all, $N = 4$ is too far from $N = \infty$. This has been previously pointed out by Kuti, et. al. [11]. More importantly, we have over estimated the decay channel of the Higgs particle in the naive large $N$ formula. At $N = 4$, the Higgs particle can decay into 3 colors of the Goldstone pairs while the large $N$ formula counts 4. When we take this into account and substitute $(N - 1)$ for $N$ in the large $N$ formula, we expect compatible results with the perturbation theory. In Figure (3.8), we have plotted the two large

![Figure 3.8](image)

**Figure 3.8**: The large $N$ results for the width of the Higgs particle as a function of the Higgs mass is shown. The open squares are the naive large $N$ prediction for $O(4)$ model. The open hexagons are the large $N$ results after the number of decay channels has been corrected. The solid line is the leading order perturbation result and the dashed line is the perturbation result up to the second order. The corrected large $N$ width agrees with the perturbative prediction very well in the weakly interacting regime as it should. The naive large $N$ result overshoots by about 30 to 40 percent.
$N$ results of the width as a function of the Higgs mass and compared them with the perturbative results. As expected, the corrected large $N$ width agrees reasonably well with the perturbative predictions, especially in the weakly interacting region or small Higgs mass. The naive large $N$ result, however, overshoots by about 30 to 40 percent simply because it fails to identify the correct number of decay channels of the Higgs particle. From this calculation, we conclude that the large $N$ approximation has its own ambiguities when it is applied to $N$ values that are not very large. Therefore, one must modify the naive large $N$ formula in order to get meaningful quantitative results.

### 3.2.4 Higgs Mass and Width for Higher Derivative $O(N)$ Model

In higher derivative theory, things are getting more complex because of the ghost pair. One could try to evaluate the continuum bubble integral in Equation (3.29) and solve for the complex pole of the Higgs propagator. Note that this integral is finite and no regulator has to be introduced. The precise form of the bubble integral is very complicated and is listed in the Appendix of this chapter. The analytic structure (Riemann sheets and cuts) are also quite complex, as described in the Appendix. The resulting function is then substituted into the full large $N$ Higgs propagator to solve for the poles. The complex pole structure of the function is also very complicated due to the existence of the ghost states. The poles are numerically searched for a given parameter $v$ in $M$ unit and a fixed value of the bare coupling constant $\lambda_0$. The result is shown in Figure (3.9). One has to be careful with the Riemann sheet structure of the function in order to get the right result. The poles are characterized by their positions on the Riemann sheets. On the first Riemann sheet, due to the ghost states, one finds a conjugate pair of poles represented by the open hexagonal points in the figure. They are moving towards the higher energy values.
Figure 3.9: The complex poles of the large $N$ Higgs propagator is shown on the first and the second Riemann sheets. The bare coupling constant is set to infinity in this figure. The open hexagonal points represent the ghost pair poles on the first Riemann sheet. The filled hexagonal points are the 'image' of the ghost on the second Riemann sheet. The filled circles are the Higgs poles on the second sheet. The size of the points reflects the different $v$ values.

These complex conjugate ghost pairs have “shadow images” on the second Riemann sheet which are represented by the filled hexagonal points. Because of the interaction with the Higgs pole on the second sheet, these poles are not moving symmetrically. The conventional Higgs poles are on the second Riemann sheet, represented by the filled circles. As the vacuum expectation value is increases in $M$ unit, the Higgs pole is moving towards the higher energy range. When the Higgs pole is at very low energy and far away from the ghost poles, the effects of the ghost states can be viewed as an effective cutoff to the conventional theory. This can also be seen in Equation (3.29). When $p^2$ is small, the bubble
integral becomes very simple and can be very well approximated by

\[ B(p^2) \sim \frac{1}{16\pi^2}(-\log(p^2) + 1/2). \] (3.37)

But, if the Higgs pole is getting closer to the energy scale of the ghost poles, the higher derivative theory feature has great importance and viewing the ghosts as the effective cutoff to the conventional theory becomes meaningless.

Identifying the real part of the Higgs pole with the mass parameter and the imaginary part with the half width, we can plot the ratio \( m_H/v \) as a function of the bare coupling constant, which is shown in Figure (3.10). In this figure, we

![Graph](image_url)

**Figure 3.10:** The large \( N \) result of the ratio \( m_H/v \) as a function of the bare coupling constant for various values of the vacuum expectation value (measured in \( M \) units) for the higher derivative \( O(N) \) theory. The maximum ratio saturates to about 4 at infinite bare coupling constant.
have selected 4 different vev values and the ratio saturates to about 4 when the bare coupling constant is brought to infinity. When we set the physical value of the vacuum expectation value to 250 GeV, this implies a Higgs particle with the mass $m_H = 1$ TeV. This should be compared with the result of the conventional $O(N)$ model discussed earlier in Figure (3.7). Although the absolute values of the Higgs mass may be somewhat ambiguous due to the large $N$ approximation, this result indicates there is a 30 percent relative increase in the Higgs mass over vev ratio when the Pauli-Villars theory is compared with the conventional $O(N)$ model on the hypercubic lattice. So we would expect the full Pauli-Villars theory should also generate a larger $m_H/v$ ratio compared with the conventional theory. Recall that the Higgs mass bound for the conventional theory is about 750 GeV (which is a ratio of 3), we expect the Pauli-Villars theory could have a heavy Higgs particle in the TeV range. In fact, this hint from the large $N$ expansion initiated our nonperturbative study of the Pauli-Villars theory [6]. As we will see in the coming chapters, this scenario of strongly interacting Higgs sector in the Pauli-Villars theory is confirmed by our nonperturbative simulation results.

We can plot the width of the Higgs particle as a function of the Higgs mass, just as we did for the conventional theory. In Figure (3.11), the similar plot for the higher derivative Pauli-Villars theory is shown. One has to again modify the naive large $N$ results for the right decay channels. At very low energy, this result agrees with the perturbative result, which means that the theory can be viewed as a Pauli-Villars regulated conventional theory. However, when the Higgs mass is getting heavier, it deviates quite rapidly from the perturbative result, and in this range, the higher derivative theory does not resemble a regulated conventional theory.
Figure 3.11: The large $N$ result for the width of the Higgs particle as a function of the Higgs mass is shown in the Pauli-Villars higher derivative $O(N)$ theory. The open squares are the naive large $N$ prediction at $N = 4$. The open hexagons are the large $N$ results after the number of decay channels has been corrected. The solid line is the leading order perturbation result and the dashed line is the perturbation result up to the second order. The corrected large $N$ width agrees with the perturbative prediction very well in the weakly interacting regime as it should. The naive large $N$ result overshoots by about 30 to 40 percent.

3.3 Perturbation Theory of the Higher Derivative $O(N)$ Model

The renormalized perturbation theory of the higher derivative scalar $O(N)$ model can be established in the usual way, except we pay special attention to the role of the ghost pair. In the low energy regime, we expect to recover the conventional theory. When the energy scale is increased, one should see the ghost pair begins to play a more important role. To incorporate this energy dependence, a mass depen-
dent renormalization scheme is needed. We now illustrate this briefly by considering the model in the broken phase.

### 3.3.1 Lagrangian and Renormalization Conditions

Let us consider the following Euclidean Lagrangian,

\[
\mathcal{L}_E = \frac{1}{2} \phi^a (-\Box - \frac{\Box^3}{M^4}) \phi^a - \frac{1}{2} \mu^2 \phi^a \phi^a + \lambda (\phi^a \phi^a)^2,
\]

\[
\delta \mathcal{L}_E = \frac{\delta Z_1}{2} \phi^a (-\Box) \phi^a + \frac{\delta Z_3}{2} \phi^a (-\frac{\Box^3}{M^4}) \phi^a - \frac{\delta \mu^2}{2} \phi^a \phi^a + \delta \lambda (\phi^a \phi^a)^2.
\]  

We can define the bare fields and bare parameters according to

\[
\phi_0^a = Z_1^{1/2} \phi^a, \quad Z_1 = 1 + \delta Z_1,
\]

\[
M_0^{-4} = \frac{Z_3}{Z_1} M^{-4}, \quad Z_3 = 1 + \delta Z_3,
\]

\[
\mu_0^2 = (\mu^2 + \delta \mu^2)/Z_1,
\]

\[
\lambda_0 = (\lambda + \delta \lambda)/Z_1^2.
\]  

Then, the total Lagrangian can be written as

\[
\mathcal{L}_{E0} = \frac{1}{2} \phi_0^a (-\Box - \frac{\Box^3}{M_0^4}) \phi_0^a - \frac{1}{2} \mu_0^2 \phi_0^a \phi_0^a + \lambda_0 (\phi_0^a \phi_0^a)^2.
\]  


In the broken phase, it is convenient to separate the Higgs field and the Goldstone fields as

$$\phi^a = \left( \begin{array}{c}
\pi^1(x) \\
. \\
. \\
. \\
. \\
\pi^{N-1}(x) \\
v + \sigma(x)
\end{array} \right)$$

(3.41)

where $v = \mu^2 / 4\lambda$ is the renormalized vev. We can then write down various propagators to one loop order and impose the following mass dependent renormalization conditions,

$$\delta v = 0,$$

$$\frac{d}{dp^2} \Gamma_{\pi\pi}(p^2)_{p^2=0} = 1,$$

$$\frac{d}{dp^2}^3 \Gamma_{\pi\pi}(p^2)_{p^2=M^2} = M^{-4},$$

$$\Gamma^{\sigma\sigma}(\kappa^2) = Z_1 \kappa^2 + Z_3 \kappa^6 / M^4 + m^2(\kappa).$$

(3.42)

Notice that the above renormalization conditions uniquely determines the four renormalized parameters. The arbitrary scale $\kappa$ is introduced to avoid the infrared divergences. All the renormalized parameters will depend on this running scale through the above definitions. It is easy to fix the counter terms according to the above
equations,

\[
\delta Z_1 = \lambda m^2 B'_{\sigma\pi}(0),
\]

\[
M^{-4} \delta Z_3 = \frac{4 \lambda m^2}{3} B''_{\sigma\pi}(M^2),
\]

\[
\frac{\delta \lambda}{\lambda^2} = 36 B_{\sigma\sigma}(\kappa^2) + 4(N - 1) B_{\pi\pi}(\kappa^2),
\]

\[
\frac{\delta m^2}{m^2} = \frac{\delta \lambda}{\lambda} + \frac{T^\sigma}{m^2} + \frac{N - 1}{3} \frac{N^\pi}{m^2},
\]

(3.43)

where the bubble integrals \(B_{\sigma\sigma}, B_{\sigma\pi}, B_{\pi\pi}\) and the tadpoles \(T^\sigma, T^\pi\) are listed below:

\[
B_{\sigma\sigma}(p^2) = \int \frac{d^4k}{(2\pi)^4} \frac{1}{(k^2 + m^2 + k^6/M^4)((k-p)^2 + m^2 + (k-p)^6/M^4)},
\]

\[
B_{\sigma\pi}(p^2) = \int \frac{d^4k}{(2\pi)^4} \frac{1}{(k^2 + m^2 + k^4/M^4)((k-p)^2 + (k-p)^6/M^4)},
\]

\[
B_{\pi\pi}(p^2) = \int \frac{d^4k}{(2\pi)^4} \frac{1}{(k^2 + k^4/M^4)((k-p)^2 + (k-p)^6/M^4)},
\]

\[
T^\sigma = \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + k^4/M^4 + m^2},
\]

\[
T^\pi = \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2 + k^4/M^4}.
\]

(3.44)

3.3.2 One-loop Mass-dependent Beta-functions

Now we can work out the one loop mass dependent \(\beta\)-function of the theory, which is obtained by noticing that the bare coupling constant \(\lambda_0\) does not depend
on the renormalization scale $\kappa$. The result can be written in the following form,

$$
\frac{1}{\lambda} \beta_\lambda = \frac{9\lambda}{2\pi^2} \left( \sum_{i,j=0}^{2} a_i a_j \int_0^1 dx \frac{x(1-x)\kappa^2}{x(1-x)\kappa^2 + x\lambda_i + (1-x)\lambda_j} \right) + \frac{N-1}{9} \sum_{i,j=0}^{2} b_i b_j \int_0^1 dx \frac{x(1-x)\kappa^2}{x(1-x)\kappa^2 + x\xi_i + (1-x)\xi_j},
$$

(3.45)

where $\hat{\kappa}^2 = \kappa^2/M^2$ and the mass parameters $\lambda_i, \xi_i$ and their corresponding residues are determined from the following decomposition:

$$
\frac{1}{k^2 + k^6 + (m/M)^2} \equiv \frac{1}{k^2 + \lambda_0} + \frac{1}{k^2 + \lambda_1} + \frac{1}{k^2 + \lambda_2},
$$

$$
\frac{1}{k^2 + k^6} \equiv \frac{1}{k^2 + \xi_0} + \frac{1}{k^2 + \xi_1} + \frac{1}{k^2 + \xi_2}.
$$

(3.46)

The important feature of these coefficients is

$$
\sum_{i=0}^{2} a_i = \sum_{i=0}^{2} b_i = 0.
$$

(3.47)

Now it is easy to see how the effective coupling constant evolve with the energy scale $\kappa$. When $\kappa/M$ is very small, the ghost pair contributions to the beta-function is negligible. The summation in the beta-function reduces to only the $i = j = 0$ contribution, which is the conventional, well-known beta-function of the $O(N)$ model in the broken phase. As $\kappa/M$ increases, the ghost contributions become increasingly important. When the energy scale is well above the ghost scale, the integral in the beta-function reduces to 1 and the quantity in the bracket vanishes due to Equation (3.47). This means that, at high energies, beta-function of the theory vanishes. Therefore, as the energy scale increases, the running coupling constant $\lambda(\kappa)$ also increases. However, at the scale of the ghost pair or higher, the coupling constant gradually flattens out to some finite number. This is a very different feature when
compared with the conventional $O(N)$ model. In the conventional $O(N)$ model, the running coupling constant keeps increasing and becomes divergent at the so-called Landau ghost energy scale. In our higher derivative theory, we have replaced the Landau ghost with real ghost pair and the running coupling constant will remain finite for all energies.

### 3.4 Appendix

In this appendix we list the explicit form of the bubble integral and discuss some analytic properties of such.

The function is given by the parametric integral representation

$$B(s) = -\frac{1}{16\pi^2} \sum_{i,j} c_ic_j \int_0^1 dx \log [xm_i^2 + (1-x)m_j^2 - x(1-x)s], \quad (3.48)$$

where the sum over $i$ and $j$ runs from 0 to 2 with the following values of $c_i$ and $m_i^2$

$$m_0^2 = 0, \quad c_0 = 1, \quad (3.49)$$

$$m_1^2 = e^{2i\Theta}, \quad c_1 = \frac{-ie^{-2i\Theta}}{2\sin 2\Theta},$$

$$m_2^2 = e^{-2i\Theta}, \quad c_2 = \frac{+ie^{2i\Theta}}{2\sin 2\Theta}.$$  

The integral can be worked out explicitly with the result

$$B(s) = -\frac{1}{16\pi^2} \left\{ c_0^2 \log(-s) + c_1^2 \left[ +2i\Theta - \frac{\sqrt{(1-s/4\mathcal{M}^2)(-s/4\mathcal{M}^2)}}{2(s/4\mathcal{M}^2)} \log\left(\frac{\sqrt{1-s/4\mathcal{M}^2 + \sqrt{-s/4\mathcal{M}^2}}}{\sqrt{1-s/4\mathcal{M}^2} - \sqrt{-s/4\mathcal{M}^2}}\right) \right] \right\}$$
\[ + c_2^2 \left[ -2i\Theta - \frac{\sqrt{(1 - s/4M^2)(-s/4M^2)}}{2(s/4M^2)} \log\left( \frac{\sqrt{1 - s/4M^2 + \sqrt{-s/4M^2}}}{\sqrt{1 - s/4M^2 - \sqrt{-s/4M^2}}} \right) \right] \]

\[ + 2c_0c_1 \left[ +2i\Theta + (1 - \frac{M^2}{s}) \log(1 - \frac{s}{M^2}) \right] \]

\[ + 2c_0c_2 \left[ -2i\Theta + (1 - \frac{M^2}{s}) \log(1 - \frac{s}{M^2}) \right] + 2c_1c_2 f(s) \tag{3.50} \]

where the last term is the ghost-antighost contribution and the function \( f(s) \) is given by

\[ f(s) = \frac{i \sin 2\Theta}{s} \left( \log\left( \frac{s - 2 \cos 2\Theta + \Delta(s)}{-2M^2} \right) + \log\left( \frac{-2M^2}{s - 2 \cos 2\Theta + \Delta(s)} \right) \right) \]

\[ - \frac{\Delta(s)}{2s} \left( \log\left( \frac{s - 2 \cos 2\Theta - \Delta(s)}{-2M^2} \right) - \log\left( \frac{s - 2 \cos 2\Theta - \Delta(s)}{-2M^2} \right) \right), \]

\[ \Delta(s) = \sqrt{(s - 4 \cos^2 \Theta)(s + 4 \sin^2 \Theta)}. \tag{3.51} \]

The logarithm functions in the above equations take the complex angle between \( \pi \) and \( -\pi \). The function \( f(s) \) was worked out long ago by Lee and Wick but our results is different from theirs [2]. Their results correspond to combining the two logarithms in the above equation, which is not always legitimate because of the restricted range of the complex phase of the arguments under the logarithms. The Riemann sheet structure of this function is highly nontrivial as shown in Figure (3.12).

Our function agrees with Lee’s function when \( Re(s) < 2 \cos 2\Theta \). The function \( f(s) \) has a cut which is a hyperbola whose center is at \((2 \cos 2\Theta, 0)\) in the complex \( s \) plane. The function \( f(s) \) has a finite jump anywhere across the cut except at \( s = 4 \cos 2\Theta \) where it is continuous. This function is analytic everywhere else away from the cut. The so-called “ghost-antighost threshold” is not a real one, and no imaginary part
contribution will arise when the center of mass energy steps through $4 \cos^2 \Theta$. This is necessary for the unitarity to hold. Other parts in the $B(s)$ function have cuts starting at the ghost pole location. In the small $s$ and large $s$ region the function $B(s)$ simplifies to

$$B(s) \xrightarrow{s \to 0} -\frac{1}{16\pi^2} \left( \log(s) - i\pi + 1/2 + O(s) \right),$$

$$B(s) \xrightarrow{s \to \infty} -\frac{1}{16\pi^2} \left( -i\pi + O(1/s) \right).$$

This concludes our discussion of the analytic properties of the function.
References

[1] A. Pais and G. E. Uhlenbeck, Phys. Rev. 79 (1950) 145.

[2] T. D. Lee and G. C. Wick, Nucl. Phys. B 9 (1969) 209; Phys. Rev. D 2 (1970) 1033.

[3] R. E. Cutkosky, P. V. Landshoff, D. I. Olive and J. C. Polkinghorne, Nucl. Phys. B12 (1969) 281.

[4] K. Jansen, J. Kuti, C. Liu Phys. Lett. B 309 (1993) 119.

[5] J. Kuti and C. Liu, to be published.

[6] K. Jansen, J. Kuti, C. Liu Phys. Lett. B309 (1993) 127.

[7] C. Liu, K. Jansen and J. Kuti, Nucl. Phys. B 34 (Proc. Suppl.), (1994) 635.

[8] M. Lüscher and P. Weisz, Phys. Lett. B212 (1988) 472.

[9] U. M. Heller, H. Neuberger and P. Vranas, Nucl. Phys. B405 (1993) 557.

[10] M. B. Einhorn, Nucl. Phys. B246 (1984) 75. M. B. Einhorn and D. N. Williams, Phys. Lett. B211 (1988) 4570.

[11] L. Lin, J. Kuti and Y. Shen, Lattice Higgs Workshop, eds. B. Berg et al. (1988) p. 186.
Chapter 4

Higher Derivative Field Theories on the Lattice

4.1 The Naive Lattice Action and Phase Diagram

The need of a lattice for the higher derivative scalar field theory presented in the previous chapter is not for the purpose of regularization, but rather, to make the degree of freedom finite so that a nonperturbative study of the model can be performed in computer simulations. The lattice spacing $a$ introduces a new short distance energy scale with the associated momentum cutoff $\Lambda = \pi/a$. In order to recover the higher derivative field theory in the continuum, we would have to work towards the $\Lambda/M \rightarrow \infty$ limit with a fixed ratio of $M/m_H$. The lattice action we choose to study [1, 2] is

$$\mathcal{L}_E = -\kappa \phi(x)(-\Box - \frac{\Box^3}{M^4})\phi(x) + (1 - 8\kappa)\phi(x)^2 - \lambda(\phi(x)^2 - 1)^2,$$

where the $\Box$ is the lattice Laplace operator. The phase structure of this lattice model is quite similar to the conventional $O(N)$ scalar field theory. It has two phases as shown in Figure (4.1). The $O(N)$ symmetric phase is separated from the broken phase with residual $O(N - 1)$ symmetry by a second order phase transition line for every value of the lattice coupling constant $\lambda$ in the $(\kappa, M)$ plane. Near the critical
Figure 4.1: The phase diagram of the lattice model at infinite bare coupling. Data points are obtained from Monte Carlo simulations. The dotted line is calculated in the large-N expansion. The solid line displays a fixed $M_R/m_H$ ratio towards the continuum limit of the higher derivative theory.

However, the critical behavior of our model is more complicated than the conventional $O(N)$ model. It can represent different universal continuum theories along different paths towards the critical line. Tuning the value of $\kappa$ towards the critical line for any fixed value of $M$ corresponds to the trivial field theory in the continuum. In this limit, the operator $\phi^{\square^3}\phi$ becomes irrelevant in the critical region. However, if we tune the value of $\kappa$ towards the critical line in such a way that the ratio $M_R/m_H$ remains fixed, we will recover the continuum higher derivative field theory with the corresponding ratio of the ghost mass parameter and the Higgs mass. In this limit the operator $\phi^{\square^3}\phi$ cannot be viewed as an irrelevant operator [4] in the Lagrangian. Thus, it becomes clear, from the discussion above, that if we want to study the higher
derivative field theory, we have to work towards the second limit.

In the practical application, however, this limit is not very easy to arrange. One reason is that if we want our results to represent the continuum results, we have to keep the ghost mass parameter $M$ reasonably small in lattice units in order to get rid of the lattice effects associated with it. On the other hand, we need to put the Higgs mass below the ghost mass parameter. Therefore, we are very restricted in the parameter space. On the one hand, making the Higgs mass smaller will lead to huge finite size effects for the practical lattice sizes; on the other hand, making the Higgs mass larger will push up the ghost mass and will result in large lattice effects. So we have a rather narrow range in the Pauli-Villars correlation length $M/m_H$. Typical values we took in the beginning of our simulation were: $M = 0.8 \sim 1.0$, $m = 0.3 \sim 0.4$. This, of course, was unsatisfactory because the ratio $M/m_H = 2 \sim 3$ is too narrow of a range. If we view this theory as a Pauli-villars regulated theory, for example, we would hope to see the conventional scaling behavior in the large $M/m_H$ limit. It turns out that the scaling form may apply only for rather large $M/m_H$ values which is impossible for us to investigate using this naive lattice action. Also, due to this restricted range, it was also impossible for us to study the scattering phase shift profile of the model. This type of analysis offers us a very good way of extracting the mass value for an unstable particle in the finite box (see Chapter 6 for full discussion). This restriction in the parameters is purely due to the introduction of the underlying lattice structure. When we were able to eliminate most of the lattice effects, we were then able to enlarge our parameter space quite substantially. Therefore, the need for an improved lattice action becomes quite obvious.
4.2 The Improved Lattice Action

Improving the lattice action so that it has better Euclidean invariance was studied long ago [3]. Our choice of the improvement corresponds to modifying the lattice Laplacian so that it resembles the continuum Laplacian. Therefore, we take

\[ p^2_I = \hat{p}^2 + a_1 \sum_\mu \hat{p}_\mu^4 + a_2 \sum_\mu \hat{p}_\mu^6 + a_3 \sum_\mu \hat{p}_\mu^8 + a_4 \sum_\mu \hat{p}_\mu^{10} + a_5 \sum_\mu \hat{p}_\mu^{12} + a_6 \sum_\mu \hat{p}_\mu^{14}, \]  

(4.2)

where the coefficients are given by the following table

|    \(a_1\) | \(a_2\) | \(a_3\) | \(a_4\) | \(a_5\) | \(a_6\) | \(a_7\) | \(a_8\) | \(a_9\) | \(a_{10}\) |
|---|---|---|---|---|---|---|---|---|---|
| \(\frac{1}{12}\) | \(\frac{1}{90}\) | \(\frac{1}{560}\) | \(\frac{1}{3150}\) | \(\frac{1}{16632}\) | \(\frac{1}{84084}\) | \(\frac{1}{411840}\) | \(\frac{1}{1969110}\) | \(\frac{1}{9237800}\) | \(\frac{1}{42678636}\) |

In fact, we calculated the renormalized coupling constant in the large \(N\) limit and we found that this improved action significantly decreased the lattice effects. With this improved lattice action, even at \(M = 2.0\), there was negligible lattice effects on the large \(N\) results. The phase diagram of the improved action is similar to the naive action.

The improved action offers us another power: the possibility of performing a phase shift simulation on the higher derivative \(O(N)\) model. This is the subject in Chapter (6). As we will demonstrate, without the improved action, we are in the parameter range that is impossible for this type of simulation because we would need unrealistically large lattices to extract the phase shift. With the improved action, this type of calculation becomes possible.
4.3 The Rotator States and Born Oppenheimer Approximation

Studying the higher derivative $O(N)$ model in the broken phase and the corresponding Higgs mass problem requires a better understanding of the symmetry breaking mechanism in the finite volume. In fact this is already an important issue in the conventional $O(N)$ theory without the higher derivative terms added. The symmetry breaking mechanism has been understood very well in the infinite volume limit. However, it has not been answered satisfactorily in the $O(N)$ model in a finite volume.

There are several complications. First of all, the notion of symmetry breaking in the infinite volume cannot be applied to a system in a finite volume. Strictly speaking, in a finite volume, the symmetry is never broken. Secondly, it turns out that the dynamics of the zeromode are crucial for the understanding, and the zeromode is coupled to other modes in a complicated way. For the one component $\phi^4$ theory, Hartree type of approximation will give us a very good description of the symmetry breaking. For the $O(N)$ model, extra care must be paid to the motion of the zeromode and new approximation schemes are needed for the understanding of the problem. This section consists of several parts. In the first part, we will review what is known to the symmetry breaking in a ordinary one-component $\phi^4$ theory in the broken phase. It turns out that this is a very instructive model to study. In the second part, the conventional $O(N)$ model is studied in the broken phase. Here we introduce the Born-Oppenheimer Approximation (or Adiabatic Approximation) and fully investigate the dynamics of the zeromode. In the third part, we consider some important applications of the Born-Oppenheimer Approximation. The machinery is applied to the ground state and higher energy excited states. The rotator correction to the energy of these states is calculated. This will serve as a theoretical guide line
to the analysis of the simulation results in Chapter (5). Then, the higher derivative \( O(N) \) theory is presented in the next section.

4.3.1 Symmetry Breaking of the One-component \( \phi^4 \) Model

Consider the one component \( \phi^4 \) theory in a cubic box. The Hamiltonian of the theory is given by

\[
\mathcal{H} = \frac{1}{2} \pi^2 + \frac{1}{2} (\nabla \phi)^2 - \frac{1}{2} \mu_0^2 \phi^2 + \lambda_0 \phi^4. \tag{4.3}
\]

This Hamiltonian is obviously invariant under the change \( \phi \rightarrow -\phi \). That is to say that one can construct a parity operator \( P \), which flips the sign of the \( \phi \) field and it commutes with the Hamiltonian. Therefore, all the eigenstates of the Hamiltonian can be chosen to have a definite parity.

We can build up two approximate ground states of the Hamiltonian \( |\pm\rangle \), which are Gaussian wavefunctions centered at \( \pm v \) respectively. This picture is very well illustrated by the so-called “Hartree approximation”. We start with a trial wave functional which is a Gaussian

\[
\Psi(\phi) = N \exp \left( -\frac{1}{2} (\phi(x) - v)G^{-1}(x,y)(\phi(y) - v) \right) \tag{4.4}
\]

where \( v, G^{-1}(x,y) \) are variational parameters and the summation over \( x \) and \( y \) is implied. The approximate ground state of the system can be found by using the minimization condition of the energy. This condition in the broken phase will give us two solutions for the parameter \( v \), namely, \( v = \pm \sqrt{\mu_0^2/4\lambda_0} \) and the propagator \( G^{-1}(x,y) \) is given by

\[
G(x, y) = \frac{1}{2} \int \frac{d^3k}{(2\pi)^3} \frac{e^{ik\cdot x}}{\sqrt{k^2 + m_R^2}} \tag{4.5}
\]
If we denote these two states as $|\pm\rangle$ then we see they satisfy the following properties

$$ P|\pm\rangle = |\mp\rangle, \quad \langle +| - \rangle = e^{-v^2mRL^3}. \quad (4.6) $$

Note that the states $|\pm\rangle$ are not orthogonal to each other in the finite volume. The true ground state and the first excited state are given by the symmetric and antisymmetric linear combination of these two states

$$ |0\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |\mp\rangle), \quad |1\rangle = \frac{1}{\sqrt{2}}(|+\rangle - |\mp\rangle). \quad (4.7) $$

The true ground state is a parity even state, while the first excited state is a parity odd state. The energy difference between the two is exponentially small when the volume is large. This means that if the system were started at one of the minimum, after a long enough time, there is a finite probability of finding the system tunneled to the other minimum. The typical time scale for this is $1/\Delta E$, where $\Delta E$ is the energy difference between the ground and the first excited state.

If we use an infinite volume, the state $|+\rangle$ would be exactly orthogonal to the state $|\mp\rangle$; then the system starting from one particular minimum of the potential as the true vacuum will stay there, without knowing the other one and the $\phi \rightarrow -\phi$ symmetry is broken. However, in a finite but large volume, the system will stay around one minimum for such a long enough time that we may say the symmetry is “almost broken”.

In the one component model, the symmetry is a discrete symmetry and the Hartree approximation gives us a very good understanding of the symmetry breaking mechanism in the finite volume. Nonperturbative works have also been done to measure the energy gap between the ground state and the first excited state, which is related to the surface tension of the system.
4.3.2 $O(N)$ Model: General Setup

The situation is much more complicated when we try to do a similar analysis for the $O(N)$ model. The main reason is that the symmetry is a continuous symmetry, therefore, the dynamics of the zeromode is much more complicated.

We could first try out the Hartree approximation, but it will not give us the right energy spectrum of the theory. This is because the Hartree approximation treats every mode of the system equally. In the one component model this is valid, but it is not valid for the $O(N)$ model. In the $O(N)$ model there exists one special mode, that is, the direction of the zero Fourier mode which can be characterized by an $O(N)$ unit vector. In a large but finite volume, this mode is a slow varying mode when compared with the other modes. It is the counterpart of the parity operator in the one component model. The only difference is that, in the one component model, the parity only takes discrete values and is not dynamical. In the $O(N)$ model, however, this unit vector lives on a $(N-1)$-sphere and has its own dynamics. Therefore, we expect that the Born-Oppenheimer Approximation (BOA), also known as the Adiabatic Approximation, will give us a very good description of the zeromode dynamics.

The Born-Oppenheimer Approximation was first introduced in the study of diatomic molecules. In the molecular problem, there are two types of degrees of freedom. The motion of the electron is called “fast”, and the motion of the nucleus is called “slow”. Therefore, when solving the energy eigenvalues of the system, one should first nail down the slow variable, namely the configuration of the nucleus, and solve the fast variable spectrum. In this step, the configuration of the slow variable is treated as an external field. The eigenvalues and eigenstates that come out will, in general, depend on the prescribed configuration of the slow variable. These eigenvalues are then taken back into the Schrödinger equation for the slow
variables as the effective potential, which reflects the feedback of the fast variable to the slow variable. Finally, the Schrödinger equation for the slow variable is solved to get the spectrum of the molecule.

The spectrum of the molecule has a three fold hierarchy: electron energy, oscillation energy and rotational energy. These energy gaps are characterized by different powers of a small parameter, which is the ratio $m_e/m_N$, where $m_e$ is the mass of the electron and $m_N$ is the mass of the nucleus. Born-Oppenheimer is a very good approximation for the molecule, since this ratio is so small. It is not hard to imagine that a Hartree approximation to the molecular problem would be a poor choice, since it treats the electron (fast variable) and the nucleus (slow variable) equally, while ignoring the enormous difference in the mass of the two. Similarly, in our application, Hartree is a poor approximation for the same reason. To get the right picture, one has to separate the special zeromode and use the Born-Oppenheimer type of approximation.

In our model, we will treat the direction of the zeromode as the only slow variable. We will use the same Born-Oppenheimer type of spirit to solve for the energy levels of our model.

We begin with the Hamiltonian

$$H = \sum_x \frac{1}{2} \pi^a \pi^a + \frac{1}{2} \nabla \phi^a \nabla \phi^a - \frac{1}{2} \mu^2 \phi^a \phi^a + \lambda_0 (\phi^a \phi^a)^2,$$

(4.8)

where for convenience we have discretize the system on a cubic lattice. The operator $\pi^a(x)$ is just the derivative operator $(-i)\partial/\partial\phi^a(x)$ in the field variable diagonal representation. Two classes of symmetry operators that commute with this Hamiltonian are very important. First, there are global $O(N)$ symmetry generators $Q^{ab}$ given by

$$Q^{ab} = \sum_x \phi^a(x) \pi^b(x) - \phi^b(x) \pi^a(x).$$

(4.9)
We also have the 3-momentum operators $P_i$
\begin{equation}
P_i = \sum_x [\phi^a(x + e_i) - \phi^a(x)]\pi^a(x),
\end{equation}
where $e_i$ is the unit vector in the $i$ direction. It is trivial to verify that these operators commute with the full Hamiltonian hence are symmetries of the theory.

We now introduce the Fourier modes of the field variable,
\begin{equation}
\phi^a(x) = \bar{\phi}^a + \frac{1}{\sqrt{V}} \sum_{k>0} \phi_k^a e^{i k \cdot x} + \phi_k^a e^{-i k \cdot x},
\end{equation}
\begin{equation}
\pi^a(x) = \frac{(-i)}{V} \frac{\partial}{\partial \bar{\phi}^a} + \frac{(-i)}{\sqrt{V}} \sum_{k>0} e^{-i k \cdot x} \frac{\partial}{\partial \phi_k^a} + e^{i k \cdot x} \frac{\partial}{\partial \phi_k^a},
\end{equation}
where $V = L^3$ is the 3-volume of the box. As we mentioned above, the zero mode $\bar{\phi}^a$ plays a very important role in the broken phase. Therefore we have singled out this mode from the nonzero momentum modes. Let us define:
\begin{equation}
\bar{\phi}^a = (v + \sigma)n^a, \quad n^a n^a = 1,
\end{equation}
\begin{equation}
P_L^{ab} = n^a n^b, \quad P_T^{ab} = \delta^{ab} - n^a n^b,
\end{equation}
where $v = \mu_0^2/4\lambda_0$ is the vev of the theory. In the Born-Oppenheimer type of approach, we will treat the direction of $\bar{\phi}^a$, namely $n^a$, as the only slow varying variable and treat the rest as fast variables. The justification of this will be seen shortly. Then the Hamiltonian can be expressed in terms of these Fourier modes.

We use the radial variables for the mode $\bar{\phi}^a$. Thus we write the wavefunctional of the system as $\Psi = \rho^{-(N-1)/2}\psi$ and the effective Hamiltonian for $\psi$ will contain only the second derivative with respect to $\rho$. For the nonzero Fourier modes, let us
introduce the creation and annihilation operators as

\[ L^a_k = \frac{1}{\sqrt{2}} P^{ab} L_L (\sqrt{\Omega_k} \phi^a_k + \frac{1}{\sqrt{\Omega_k}} \partial \phi^b_k), \]

\[ L^{a\dagger}_k = \frac{1}{\sqrt{2}} P^{ab} L_L (\sqrt{\Omega_k} \phi^{a\ast}_k - \frac{1}{\sqrt{\Omega_k}} \partial \phi^b_k), \]

\[ L^a_{-k} = \frac{1}{\sqrt{2}} P^{ab} L_L (\sqrt{\Omega_k} \phi^a_k + \frac{1}{\sqrt{\Omega_k}} \partial \phi^b_k), \]

\[ L^{a\dagger}_{-k} = \frac{1}{\sqrt{2}} P^{ab} L_L (\sqrt{\Omega_k} \phi^{a\ast}_k + \frac{1}{\sqrt{\Omega_k}} \partial \phi^b_k), \] (4.13)

where \( \Omega_k = \sqrt{m_0^2 + k^2} \) is the higgs excitation. We can define the Higgs creation and annihilation operators as

\[ h_k = n^a L^a_k, \quad h^{\dagger}_k = n^a L^{a\dagger}_k, \quad \sigma = \frac{1}{\sqrt{2V m_0}} (h_0 + h^{\dagger}_0). \] (4.14)

Similarly, we can define the transverse Goldstone creation and annihilation operators as

\[ T^a_k = \frac{1}{\sqrt{2}} P^{ab} T_T (\sqrt{\omega_k} \phi^a_k + \frac{1}{\sqrt{\omega_k}} \partial \phi^b_k), \]

\[ T^{a\dagger}_k = \frac{1}{\sqrt{2}} P^{ab} T_T (\sqrt{\omega_k} \phi^{a\ast}_k - \frac{1}{\sqrt{\omega_k}} \partial \phi^b_k), \]

\[ T^a_{-k} = \frac{1}{\sqrt{2}} P^{ab} T_T (\sqrt{\omega_k} \phi^a_k + \frac{1}{\sqrt{\omega_k}} \partial \phi^b_k), \]

\[ T^{a\dagger}_{-k} = \frac{1}{\sqrt{2}} P^{ab} T_T (\sqrt{\omega_k} \phi^{a\ast}_k + \frac{1}{\sqrt{\omega_k}} \partial \phi^b_k), \] (4.15)

where \( \omega_k = |k| \) is the Goldstone energy. In terms of these operators, we can rewrite
the effective Hamiltonian in the following form

\[ H = \sum_k \Omega_k h_k^\dagger h_k + \sum_{k \neq 0} \omega_k T_k^a T_k^a + H_{\text{int}} + \frac{L^2 + \Delta_N}{2V(u + \sigma)^2}, \]

\[ H_{\text{int}} = \sum_x 4\lambda_0 v(h^2 + \tilde{\phi}_T^a \tilde{\phi}_T^a) + \lambda_0 (h^2 + \tilde{\phi}_T^a \tilde{\phi}_T^a)^2, \]  \( (4.16) \)

where the fields \( h(x) \) and \( \tilde{\phi}_T^a \) are given by

\[ h(x) = \sum_k \frac{1}{\sqrt{2\Omega_k}} (h_k e^{ik \cdot x} + h_k^\dagger e^{-ik \cdot x}), \]

\[ \tilde{\phi}_T^a(x) = \sum_{k \neq 0} \frac{1}{\sqrt{2\omega_k}} (T_k e^{ik \cdot x} + T_k^\dagger e^{-ik \cdot x}), \]  \( (4.17) \)

and the constant \( \Delta_N = (N - 3)(N - 1)/4 \). The operator \( L^2 \equiv L_0^{ab} L_0^{ab}/2 \) is the \( O(N) \) Casimir of the zeromode variable. The above creation and annihilation operators satisfy the following commutation relations

\[ [T_k^a, T_p^{b\dagger}] = P_T^{ab} \delta_{kp}, \quad [L_k^a, L_p^{b\dagger}] = P_L^{ab} \delta_{kp}. \]  \( (4.18) \)

It is also very convenient to introduce the following decomposition for the fields. For a given \( O(N) \) unit vector \( n^a \), we can find additional \( N - 1 \) unit vectors which, together with \( n^a \), form a complete set in the \( O(N) \) space. We therefore define

\[ n_0^a \equiv n^a, \quad n_\alpha^a n_\beta^a = \delta_{\alpha\beta}, \quad \alpha, \beta = 0, 1, ... N - 1, \]

\[ T_k^a = n_i^a T_{ik}, \quad T_{ik} = n_i^0 T_k^a, \]

\[ L_k^a = n_0^a h_k, \quad h_k = n_0^0 L_k^a. \]  \( (4.19) \)
It is readily checked that these operators satisfy the standard commutation relations

\[ [h_k, h^\dagger_p] = \delta_{kp}, \quad [T_{ik}, T^\dagger_{jp}] = \delta_{ij}\delta_{kp}. \]  

(4.20)

Note that due to the leftover $O(N - 1)$ symmetry, the determination of the unit vectors $n^a_i$ is not unique. However, the physical quantities will not depend on this ambiguity. Moreover we can calculate the commutator of the operator $L_0^{ab}$ with the unit vectors,

\[ [L_0^{ab}, n^c_i] = (-i)n^a_\alpha \delta^{bc}_\alpha, \quad \alpha = 0, 1, \ldots N - 1. \]  

(4.21)

Now we can set up a basis in our Hilbert space from the eigenstate of the free Hamiltonian. We will also choose the angular momentum eigenstate of the $n^a$ variable, namely

\[ |n, \{n^L_k, n^T_k\}, lm\rangle = |n\rangle \otimes \prod_{k \neq 0} |n^L_k\rangle \otimes |n^T_k\rangle \otimes |lm\rangle, \]  

(4.22)

where the state $|lm\rangle$ is the eigenstate of $L^2$ with eigenvalue $l(l + N - 1)$. This is just a symbolic notation of the state. Strictly speaking, for $O(N)$ model, we need more quantum numbers to specify the state. Note that the oscillator part of the state actually depends on the unit vector $n^a$ via the definition of the longitudinal and transverse projection, although the eigenvalue does not. Therefore, if we were to act the operator $L^2$ on the states above, it would not only act on the state $|lm\rangle$, but also act on the rest of the components ( except $|n\rangle$, of course, since it is the radial zero momentum mode ). As we will see below, the Born-Oppenheimer Approximation will first neglect the effect of $L^2$ on the fast modes and only consider the slow mode part of the state, i.e. $|lm\rangle$. The next order correction has to take this into account and the BOA is valid when the correction is small.

The global $O(N)$ generator $Q^{ab}$ now can be expressed in terms of the creation
and annihilation operators defined in Equation (4.19)

\[ Q^{ab} = L^{ab}_0 - i \sum_{k \neq 0} T^\dagger_{0k} T_{0k} n^{[a}_0 n^{b]}_0, \]  

(4.23)

where the index \( \alpha \) and \( \beta \) run from 0 to \((N - 1)\). The operators \( T_{0k} \) and the functions \( f_k, g_k \) are defined by the following:

\[ T^\dagger_{0k} = f_k h_k^\dagger - g_k h_{-k}, \quad T_{0k} = f_k h_k - g_k h_{-k}, \]

\[ f_k = \frac{1}{2} \left( \sqrt{\Omega_k / \omega_k} + \sqrt{\omega_k / \Omega_k} \right), \quad g_k = \frac{1}{2} \left( \sqrt{\Omega_k / \omega_k} - \sqrt{\omega_k / \Omega_k} \right). \]  

(4.24)

We will need the result of \( L^2 \) acting on the oscillator states. Let us consider the object \( L^2 |0_{k \neq 0} \rangle \). This can be easily obtained by noticing that the state is annihilated by the global \( O(N) \) generators \( Q^{ab} \). Therefore we would induce that

\[ L^{ab}_0 |0_{k \neq 0} \rangle = \sum_{k \neq 0} i g_k n^{[a}_0 n^{b]}_i h^\dagger_{-k} T^\dagger_{ik} |0_{k \neq 0} \rangle. \]  

(4.25)

We will also need the commutation relations between \( L^{ab}_0 \) and the annihilation operators

\[ [L^{ab}_0, L^c_k] = (-i) n^{[a}_0 n^{b]}_c h_k + n^c (f_k n^{[a}_k T^{b]}_k + g_k n^{[a}_k T^{b]}_{-k}), \]

\[ [L^{ab}_0, T^c_k] = (-i) n^{[a}_0 n^{b]}_c (f_k h_k - g_k h^\dagger_{-k}) + n^c n^{[a}_k T^{b]}_{-k}, \]  

(4.26)

or equivalently, in terms of operators \( T_{ik} \) and \( h_k \), we have

\[ [L^{ab}_0, h_k] = (-i) n^{[a}_0 n^{b]}_i (f_k T_{ik} + g_k T^\dagger_{i-k}), \]

\[ [L^{ab}_0, T_{ik}] = (-i) n^{[a}_i n^{b]}_j T_{jk} + (-i) n^{[a}_0 n^{b]}_i (f_k h_k - g_k h^\dagger_{-k}). \]  

(4.27)

The corresponding commutators with the creation operators can be obtained from
hermitian conjugation of the above equations. We now have all the tools to study
the rotator energy spectrum.

4.3.3 $O(N)$ Model: The Ground States

The full ground state of the free Hamiltonian consists of two parts. One is
the ground state of oscillator states. The other part is the rotator states.

$$|G, lm\rangle = |0_{osc}\rangle \otimes |lm\rangle.$$  \hspace{1cm} (4.28)

Note that, before the rotator energy contributions are taken into account, the de-
generacy of the ground state is infinite, since any rotator state $|lm\rangle$ will belong to
the same energy. It is very easy to check that all these states are eigenstates of the
momentum operator with eigenvalue of 0. They can also be taken as the eigenstates
of the appropriate $O(N)$ operators. To see this, notice that when the operator $Q_{ab}$
is applied to the states, it generally has two contributions. One is from $Q_{ab}$ acting
on the oscillator state $|0_{osc}\rangle$, which is zero in this case; the other is from $Q_{ab}$ acting
on the rotator states $|lm\rangle$, which is equivalent to $L_{0}^{ab}|lm\rangle$. Therefore, we have

$$Q_{ab}|G, lm\rangle = |0_{osc}\rangle \otimes L_{0}^{ab}|lm\rangle.$$  \hspace{1cm} (4.29)

By taking the states $|lm\rangle$ to be the eigenstates of the zeromode Casimir, we also make
the ground states to have the appropriate $O(N)$ charges. Basically, the oscillator
ground state has $O(N)$ charge 0, and all the $O(N)$ charges comes from the rotator
states.

As mentioned above, the leading order ground states are infinitely degenerate
due to the rotator states. This degeneracy is lifted once the first nonvanishing rotator
correction is taken into account. To do this, let us evaluate the matrix element of
the rotator energy operator \((1/2)L_{0}^{ab}L_{0}^{ab}\omega_{r}\) among the ground states

\[
L_{0}^{ab}|0_{osc}\rangle \otimes |lm\rangle = (L_{0}^{ab}|0_{osc}\rangle) \otimes |lm\rangle + |0_{osc}\rangle \otimes (L_{0}^{ab}|lm\rangle),
\]

where we have used Equation (4.25). Therefore we get

\[
\langle G,l'm'|1/2L_{0}^{ab}L_{0}^{ab}\omega_{r}|G,lm\rangle = \left[l(l + N - 2)\omega_{r} + (N - 1)\omega_{r} \sum_{k} g_{k}^{2}\right] \delta_{ll'} \delta_{mm'}.
\]

As expected, the degeneracy is lifted, and the ground states now have a degeneracy of \(l^{2}\), for a given \(l\) value. The second term in the above equation is an \(l\) independent constant and can be absorbed into the definition of the ground state energy. The first term is \(l\) dependent and is known as the rotator energy spectrum. This formula was derived before by Leutwyler using the rigid rotator approximation in the chiral Lagrangian formalism. The significance of this energy spectrum in the Monte Carlo simulation was also discussed [5]. The low energy excitations of the model exhibit a three hierarchy of energy gaps. The largest energy gap is the mass gap of the Higgs particle, whose energy is independent of the 3-volume. The second largest gap is the Goldstone particle, whose energy gap is typically of order \(O(1/L)\), where \(L\) is the size of the 3 dimensional cubic box. The smallest gap is the rotator energy differences between different \(l\) values, whose energy is of order \(O(1/L^{3})\). In a practical simulation, the size of the Higgs gap and the Goldstone energy gap are of the same order, since the size of the box is not large enough. However, the energy gap of the rotator is usually much smaller compared with the Higgs and Goldstone. Therefore we expect the Born-Oppenheimer picture should be a very good description of the theory in the finite box.

It is also possible to evaluate the second order correction to the ground state
energy. Let us first look at the following quantity

\[
L^a_0 L^b_0 |G, lm\rangle = (L^a_0 L^b_0 |0_{osc}\rangle) \otimes |lm\rangle + 2(L^a_0 |0_{osc}\rangle \otimes (L^b_0 |lm\rangle) + |0_{osc}\rangle \otimes (L^a_0 L^b_0 |lm\rangle). \tag{4.32}
\]

The first term in the above equation will contribute at the second order but it is a term independent of \(l\). If we only focus on the \(l\)-dependent terms, we can forget about this term. The last term is diagonal, it will not contribute to the second order correction of the ground state energy. Therefore, only the second term will give us \(l\)-dependent contribution to the ground state energy. The state left over is

\[
2(L^a_0 |0_{osc}\rangle \otimes (L^b_0 |lm\rangle) = 2 \sum_{k \neq 0, a, b, i} g_k n^a_0 n^b_i h^\dagger_k r^\dagger_{i-k} |0_{osc}\rangle \otimes (L^a_0 L^b_0 |lm\rangle). \tag{4.33}
\]

Therefore, it will contribute a second order energy correction that looks like

\[
E^{(2)}_{0l} = - \sum_{k \neq 0, i} \frac{\omega_r g_k^2}{\omega_k + \Omega_k} \langle lm| L^c d \n^b_0 \n^a_i \n^d_0 \n^c_0 L^a_0 \otimes |lm\rangle. \tag{4.34}
\]

The matrix element that appears in the above equation can be simplified by noticing

\[
L^c d \n^b_0 \n^a_i \n^d_0 \n^c_0 L^a_0 = 4 L^a_0 \n^b_0 \n^c_0 L^a_0 . \tag{4.35}
\]

We can pick our \(O(N)\) axis such that the unit vector is in the direction \((0, 0, \cdots, 1)\). Then the above operator simplifies to the difference of two Casimirs: the Casimir of the \(O(N)\) and the Casimir of the unbroken \(O(N - 1)\)

\[
E^{(2)}_{0l} = - \sum_{k \neq 0} \frac{2\omega_r^2 g_k^2}{\omega_k + \Omega_k} \left( l(l + N - 2) - \langle lm| L^2_{O(N-1)} |lm\rangle \right). \tag{4.36}
\]

This correction is usually very small for practical simulation parameters. However, there is another second order correction of the rotator Hamiltonian. Recall that we
can expand the rotator Hamiltonian into the form
\[
\frac{L^2 + \Delta_N}{2V(v + \sigma)^2} = \frac{L^2 + \Delta_N}{2Vv^2}(1 - \frac{2\sigma}{v} + \frac{3\sigma^2}{v^2} + \ldots). \tag{4.37}
\]

Note that the operator \( \sigma = (h_0 + h_0^\dagger) / \sqrt{2Vm_0} \). Therefore we have a systematic expansion in inverse powers of the 3-volume. If we introduce the rotator energy \( \omega_r \equiv 1/2Vv^2 \), then we have an expansion in terms of the small quantity \( \omega_r/m \). Therefore, there is another contribution from the operator \( L^2\omega_r(\sigma/v)^2 \) which is also of the order of \( \omega_r^2 \). So we have
\[
E_{nl}^{(0)} = (n + 1/2)m, \\
E_{nl}^{(1)} = [(l(l + N - 2) + \Delta_N] \omega_r, \\
E_{nl}^{(2)} = (l(l + N - 2) + \Delta_N) \omega_r (n + 1/2) \frac{6\omega_r}{m}.
\]

The first term basically takes into account the nonrigid effects of the rotator.

4.3.4 \( O(N) \) Model: The Zero Momentum Higgs States

Let us consider the energy corrections to the state \( |n, 0_{k\neq0}, lm\rangle \). Since the zero momentum Higgs excitation is just the radial excitation which commute with the angular variables. Therefore the energy corrections to the state are very much like the corrections for the ground states.
\[
E_{nl}^{(0)} = (n + 1/2)m, \\
E_{nl}^{(1)} = [(l(l + N - 2) + \Delta_N] \omega_r, \\
E_{nl}^{(2)} = (l(l + N - 2) + \Delta_N) \omega_r (n + 1/2) \frac{6\omega_r}{m}.
\]
\[- \sum_{k \neq 0} \frac{2 \omega_r^2 g_k^2}{\omega_k + \Omega_k} \left( l(l + N - 2) - \langle lm | L^2_{O(N-1)} | lm \rangle \right). \quad (4.39)\]

The second order correction is down by an extra factor of $\omega_r/m$ compared with the first order correction. However, due to the large numerical factor in front, the effect of the first term is still quite significant. In a practical simulation, the correlation function $\langle n^a(0)n^a(\tau) \rangle$ is measured and used as a way of extracting the vacuum expectation value $v$. This correlation function will pick up the energy difference of $\Delta l = 1$ states. In most of the old simulations on $O(4)$, the ratio $\omega_r/m$ is very small and the rigid approximation of the rotator energy gives very reliable results. In our recent simulations on the higher derivative theories, this ratio is of the order of 10 percent and the correction is noticeable. We would find the wrong $v$ value if we did not include this correction.

### 4.3.5 $O(N)$ Model: Two Pion States

We can perform the similar calculation for the two pion states. Let us take the isospin zero channel states $(N - 1)^{-1/2} T_{i,k}^\dagger T_{i,-k}^\dagger |0\rangle \otimes |lm\rangle$. We have

\[
\langle l'm'| \otimes \langle 0| T_{i,k} T_{i,-k} L^2 \omega_r T_{i,k}^\dagger T_{i,-k}^\dagger |0\rangle \otimes |lm\rangle / (N - 1)
\]

\[= \left( l(l + N - 2) + (N - 1) \sum_{p \neq 0} q_p^2 + 2f_k^2 + 2g_k^2 \right) \omega_r \delta_{wm}. \quad (4.40)\]

which implies that relative to the ground state the finite volume correction is

\[\Delta(2\omega_k) = 2(f_k^2 + g_k^2) \omega_r. \quad (4.41)\]

This correction is also very small when we extract the two pion energy. For the simulation points where we extract the two pion energies, this correction is below 1 percent and is therefore hidden in the statistical errors.
4.4 Symmetry Breaking of the Higher Derivative $O(N)$ Model

The similar analysis can be done with the higher derivative $O(N)$ model. Having discussed the ordinary $O(N)$ theory we will be very brief and only point out the differences. Many steps are also similar to the quantization of the higher derivative theory which was discussed in detail in Chapter (2).

One starts with the general higher derivative Lagrangian which has a global $O(N)$ symmetry

\[ \mathcal{L} = \frac{1}{2} \phi^a (-\rho_1 \Box - \rho_2 \Box^2 - \rho_3 \Box^3) \phi^a + \frac{1}{2} \mu_0^2 \phi^a \phi^a - \lambda_0 (\phi^a \phi^a)^2, \]  

(4.42)

where $\Box = \partial_t^2 - \nabla^2$ is the Minkowski space d’Alambert operator and the coefficients are parametrized as

\[ \rho_1 = 1 + \frac{m_0^2}{\mathcal{M}^2} + \frac{m_0^2}{\mathcal{M}^2}, \quad \rho_2 = \frac{1}{\mathcal{M}^2} + \frac{1}{\mathcal{M}^2} + \frac{m_0^2}{\mathcal{M}^2}, \quad \rho_3 = \frac{1}{\mathcal{M}^2 \mathcal{M}^2}. \]  

(4.43)

After the usual steps of indefinite metric quantization, and introduction of the Fourier modes, the Hamiltonian has the form (see Equation (2.50) to Equation (2.53) for detail)

\[ H = \frac{1}{V} \left( i \pi_{10}^a \pi_{20}^a + \frac{1}{2 \rho_3} \pi_{30}^a \pi_{30}^a + \frac{\rho_1}{2} \pi_{20}^a \pi_{20}^a \right) + V \left( \frac{\rho_2}{2} \tilde{\phi}_3^a \tilde{\phi}_3^a + i \tilde{\phi}_2^a \tilde{\phi}_3^a \right) \]

\[ + \sum_{k>0} i \pi_{1k}^a \pi_{2k}^a + i \pi_{1k}^a \pi_{2k}^a + \frac{1}{\rho_3} \pi_{3k}^a \pi_{3k}^a + (\rho_1 + 2 \rho_2 k^2 + 3 \rho_3 k^4) \pi_{2k}^a \pi_{2k}^a \]

\[ + (\rho_1 k^2 + \rho_2 k^4 + \rho_3 k^6) \phi_{1k}^a \phi_{1k}^a + (\rho_2 k^4 + 3 \rho_3 k^2) \phi_{3k}^a \phi_{3k}^a + i \phi_{2k}^a \phi_{3k}^a + i \phi_{2k}^a \phi_{3k}^a \]

\[ - \sum_x \frac{1}{2} \mu_0^2 \phi_1^a \phi_1^a + \sum_x \lambda_0 (\phi_1^a \phi_1^a)^2. \]  

(4.44)
Because we are now treating the system in a finite volume, we can no longer neglect the motion of the zeromode. Instead, following the idea of Born-Oppenheimer Approximation (or Adiabatic Approximation), we will single out the direction of the $\bar{\phi}_1^a$ variable and make it the slow variable in our Born-Oppenheimer approximation. We can then decompose

$$\phi_1^a = vn^a + h(x)n^a + \tilde{\phi}_1^a(x),$$

and similarly for the $\phi_2$ and $\phi_3$ variables. The Hamiltonian is then written as sum of three types of terms

$$H = H_0 + H_{k\neq 0} + H_{\text{int}},$$

$$H_0 = \frac{1}{V}(i\pi_{10}^a\pi_{20}^a + \frac{1}{2\rho_3}\pi_{30}^a\pi_{30}^a + \frac{\rho_1}{2}\pi_{20}^a\pi_{20}^a) + V(\frac{\rho_2}{2}\bar{\phi}_3^a\bar{\phi}_3^a + i\bar{\phi}_2^a\bar{\phi}_3^a + \frac{m_0^2}{2}\sigma^2),$$

$$H_{k\neq 0} = \sum_{k>0} i\pi_{1k}^a\pi_{2k}^{a*} + i\pi_{1k}^{a*}\pi_{2k}^a + \frac{1}{\rho_3}\pi_{3k}^a\bar{\pi}_{3k}^{a*} + (\rho_1 + 2\rho_2k^2 + 3\rho_3k^4)\pi_{2k}^a\bar{\pi}_{2k}^{a*}$$

$$+ (\rho_1k^2 + \rho_2k^4 + \rho_3k^6 + m_0^2)\bar{\phi}_{1kL}^a\bar{\phi}_{1kL}^{a*} + (\rho_1k^2 + \rho_2k^4 + \rho_3k^6)\bar{\phi}_{1kT}^a\bar{\phi}_{1kT}^{a*}$$

$$+ (\rho_2 + 3\rho_3k^2)\bar{\phi}_{3k}^a\bar{\phi}_{3k}^{a*} + i\bar{\phi}_{2k}^a\bar{\phi}_{3k}^{a*} + i\bar{\phi}_{3k}^a\bar{\phi}_{2k}^{a*},$$

$$H_{\text{int}} = \sum_x 4\lambda_0vh(h^2 + \bar{\phi}_{1T}^a\bar{\phi}_{1T}^a) + \lambda_0(h^2 + \bar{\phi}_{1T}^a\bar{\phi}_{1T}^a)^2. \quad (4.46)$$

This Hamiltonian is identical to what we had in Chapter (2), except for the $H_0$ piece (see Equation (2.55)). For example, the $k \neq 0$ piece can be diagonalized in the same way as in Chapter (2). The interaction piece is also expressed as the creation and annihilation operators through the field variables. The $H_0$ piece can be decomposed as follows in the finite volume. For convenience we use the rescaled variables given
by

$$p_1^a = (\rho_1 V)^{-1/2} \pi_{10}^a, \quad p_2^a = \sqrt{\frac{\rho_1 V}{\pi_{20}^a}} \pi_{20}^a, \quad p_3^a = (\rho_3 V)^{-1/2} \pi_{30}^a,$$

$$q_1^a = (\rho_1 V)^{1/2} \phi_1^a, \quad q_2^a = \sqrt{\frac{V}{\rho_1}} \phi_2^a, \quad q_3^a = (\rho_3 V)^{1/2} \phi_3^a,$$

(4.47)

and use the radial variables for $q_i^a$

$$q_1^a = \sqrt{\rho_1 V} (v + \sigma) n^a = \rho n^a.$$

(4.48)

The derivatives for the $q_i^a$ are now substituted by

$$\frac{\partial}{\partial q_i^a} = n^a \frac{\partial}{\partial \rho} + (\delta^{a\alpha} - n^a n^\alpha) \frac{\partial}{\partial n^\alpha},$$

(4.49)

where the index $a$ runs from 1 to $N$ while the index $\alpha$ only runs from 1 to $N - 1$.

The main difference lies in the derivative term with respect to the rotator variable $n^a$. In Chapter (2), this was neglected because we were in the infinite volume. This term practically serves as the kinetic energy of the zeromode variable $n^a$. One can establish the following identity

$$ip_1^a p_2^a = ip_2 L p_1 - ip_2^b n^b L_0^{ab},$$

(4.50)

where $L_0^{ab}$ is the generator of the variable $q_i^a$ only, i.e.,

$$L_0^{ab} = (-i)(q_1^a \frac{\partial}{\partial q_1^b} - q_1^b \frac{\partial}{\partial q_1^a}).$$

(4.51)

With these transformations, $H_0$ is further decomposed into three parts

$$H_0 = H_{0L} + H_{0T} + H_{0LT}$$

$$H_{0L} = ip_2 L y + \frac{1}{2} p_2^2 L + \frac{1}{2} q_3^2 L + \frac{2}{\rho_3} q_3^2 L + i \sqrt{\frac{\rho_1}{\rho_3}} q_2 L q_3 L + \frac{m_0^2}{2 \rho_1} y^2,$$
\begin{align*}
H_{0T} &= \frac{1}{2} p_{2T}^a p_{2T}^a + \frac{1}{2} p_{3T}^a p_{3T}^a + \rho_2 q_{3T}^a q_{3T}^a + \frac{\rho_1}{\rho_3} q_{2T}^a q_{3T}^a, \\
H_{0LT} &= (-i) p_{2T}^a \frac{n^b}{\rho} L_{0}^{ab}. \quad (4.52)
\end{align*}

The longitudinal part has the same form as the simple oscillator and can be diagonalized easily. The transverse part can also be diagonalized as shown in Chapter (2)

\begin{align*}
H_{0T} &= \sum_{i \neq 0, a} a_{i 0T}^{(+a)} a_{i 0T}^{(-a)} \omega_{i 0T}^{a} \quad (4.53)
\end{align*}

where the summation of \( a \) is from 1 to \( N \) and the energy gap is \( \omega_{10T} = \mathcal{M}_g \) and \( \omega_{20T} = \mathcal{M}_g \). In terms of these operators we can write out the explicit form of \( p_{2T}^a \)

\begin{align*}
p_{2T}^a &= \sum_{i \neq 0} \sqrt{\frac{\omega_{i 0T}}{2}} \epsilon_i (a_{i 0T}^{(-a)} - a_{i 0T}^{(+a)}), \quad (4.54)
\end{align*}

where the polarization factor \( \epsilon_i \) is given by \( \epsilon_1 = \epsilon_2 = i/(1 - e^{-4i \theta_g})^{1/2} \).

To summarize, in the finite volume we would have the following Hamiltonian

\begin{align*}
H &= H_0 + H_{\text{int}} + \frac{(-i)}{2} \left( p_{2T}^a \frac{n^b}{\rho} L_{0}^{ab} + \frac{n^b}{\rho} L_{0}^{ab} p_{2T}^a \right), \\
H_0 &= \sum_{i, k, \lambda} a_{i k \lambda}^{(+a)} a_{i k \lambda}^{(-a)} \omega_{i k \lambda}, \\
H_{\text{int}} &= \sum_{x} 4\lambda_0 \nu \hbar (\phi_1^a \tilde{\phi}_1^a) + \lambda_0 (\hbar^2 + \tilde{\phi}_1^a \phi_1^a)^2. \quad (4.55)
\end{align*}

In this expression, the first two terms are just the Hamiltonian of the model in the broken phase in the infinite volume. The third term is a purely finite volume correction which describes the coupling between the zeromode and the rest of degrees of freedom. The index \( \lambda \) takes the value \( L \) and \( T \) respectively. All the operators can
be expressed in terms of the creation and annihilation operators as

\[
h(x) = \sum_{i,k} \frac{c_{iL}}{\sqrt{2\omega_{ikL}}} \left( n^a_{iL} a_{iL}^a e^{ikx} + n^a_{iL} a_{iL}^a e^{-ikx} \right),
\]

\[
\tilde{\phi}^a_T(x) = \sum_{i,k \neq 0} \frac{c_{iT}}{\sqrt{2\omega_{ikT}}} \left( a_{iT}^a e^{ikx} + a_{iT}^a e^{-ikx} \right), \tag{4.56}
\]

\[
\rho = \sqrt{\rho_1 V (v + \sigma)} = \sqrt{\rho_1 V} \left( v + \sum_i \frac{c_{iL}}{\sqrt{2\omega_{i0L}}} (a_{i0L} - a_{i0L}^+) \right),
\]

where the form factors \(c_{i\lambda}\) are given by the following table

\[
c_{0L} = \sqrt{\frac{\mathcal{M}^2 \mathcal{M}^2}{(m_0^2 - \mathcal{M}^2)(m_0^2 - \mathcal{M}^2)}}, \quad c_{1L} = c_{2L} = \sqrt{\frac{\mathcal{M}^2 \mathcal{M}^2}{(\mathcal{M}^2 - m_0^2)(\mathcal{M}^2 - \mathcal{M}^2)}},
\]

\[
c_{0L} = 1, \quad c_{1T} = c_{2T} = \sqrt{\frac{\mathcal{M}_g^2}{(\mathcal{M}_g^2 - \mathcal{M}_g^2)}}. \tag{4.57}
\]

The creation and annihilation operators enjoy the following commutation relations

\[
[a_{i\lambda}^a, a_{j\lambda'}^b] = \delta_{ij} \delta_{kp} \delta_{\lambda\lambda'} P_{\lambda}^{ab}. \tag{4.58}
\]

In the higher derivative model we have the similar relation for the \(O(N)\) generators acting on the ground state

\[
L_0^{ab}|0\rangle = i \sum_{i,k \neq 0} g_{ik} a_{iL}^{(+a} a_{ikT}^{|0\rangle}.
\tag{4.59}
\]

With these relations we can now calculate the rotator contribution to the energy of the state. Due to the selection rule for the operator \(p_{2T}^0\), the first order correction vanishes. The lowest order correction comes in at the second order in the perturbation Hamiltonian. Using the representations of the operators in terms of the creation and annihilation operators, it is easy to show that the first correction is simply the
rotator energy,

\[ E_{0l}^{(1)} = [l(l + N - 2) + \Delta_N] \omega_r. \]  

(4.60)

Therefore, just like in the conventional \( O(N) \) model in the broken phase, the rotator energy spectrum is the most densely spaced excitation and dominates the invariant correlation functions.
References

[1] K. Jansen, J. Kuti, C. Liu Phys. Lett. B309 (1993) 127.

[2] C. Liu, K. Jansen and J. Kuti, Nucl. Phys. B 34 (Proc. Suppl.), (1994) 635.

[3] K. Symanzik, Nucl. Phys. B226 (1983) 187.

[4] U. M. Heller, H. Neuberger and P. Vranas, Nucl. Phys. B405 (1993) 557.

[5] A. Hasenfratz et al., Nucl. Phys. B356 (1991) 332.
Chapter 5

Simulation Results and Discussions

5.1 Simulation Algorithms

Finding the right algorithms for the higher derivative $O(N)$ model has been quite tricky [5, 6]. In the beginning of this project, we ran many tests on the existing algorithms for our model. First we tried some conventional update algorithms, for example: metropolis, heatbath and hybrid Monte Carlo. But these type of algorithms had several serious problems. One of these problems was that due to the next-next nearest neighbor coupling terms in our model, the neighbor gathering process becomes a rather time consuming task. In four dimensions, with the naive discretization, we would have had to collect the field variables at 128 neighbors for every lattice point. Compared with the ordinary theory, this is a factor of 16 more. Another problem of such algorithms was the critical slowing down when close to the criticality. This second problem was understandable because, in our model, the spectrum of the Fourier modes is greatly broadened by the higher derivative term. To understand more about this issue, let us look at the autocorrelation time in a standard hybrid Monte Carlo algorithm.

Consider the higher derivative free field theory governed by the Euclidean
Lagrangian

\[ L_E = \sum_p \omega_p^2 \phi(p) \bar{\phi}(-p), \]

(5.1)

where the spectrum \( \omega_p^2 = p^2 + p^6/M^4 + m_0^2 \). The acceptance and autocorrelations in this Gaussian type of hybrid Monte Carlo has been studied by A. D. Kennedy et. al. [1]. The autocorrelation time of the algorithm was found to be:

\[ \tau = \frac{2\tau_0}{1 - \sqrt{1 - (2\omega_{\min}\tau_0)^2}}, \]

(5.2)

where \( \tau_0 \) is the average length of each hybrid trajectory. The quantity \( \omega_{\min} \) is the lowest frequency of the Fourier modes, i.e. \( \omega_{\min} = \min_p \omega_p \). The minimum of the autocorrelation time is obtained when \( \tau_0 = 1/(2\omega_{\min}) \) with the value \( \tau = 1/\omega_{\min} \). For the stability of the leapfrog integration scheme, the step size cannot exceed \( (1/\omega_{\max}) \), where \( \omega_{\max} = \max_p \omega_p \) is the highest frequency of the Fourier modes. Therefore, the computer time that the algorithm consumes to generate an independent configuration is given by

\[ T_{\text{comp}} \sim \frac{\omega_{\max}}{\omega_{\min}}. \]

(5.3)

Thus, the computer time needed to generate an independent configuration greatly depends on how broad the extent of the spectrum. In the conventional model, the highest frequency is given by \( \omega_{\max} = \sqrt{16 + m^2} \). The lowest frequency is just \( m \). With the higher derivative term added, the extension of this frequency is much broader than the former case. The highest frequency changes to \( \omega_{\max} = \sqrt{16 + (16/M^2)^3 + m^2} \) while the lowest frequency remains unchanged. For the parameter range of \( M \) where we perform our simulation, this highest frequency is larger by a factor of 10 or more. Therefore, the autocorrelation time is enormous for the higher derivative theory in standard hybrid Monte Carlo due to the broadening effect of the frequency.
For the Gaussian model, this effect can be overcome by the so-called Fourier acceleration procedure [2, 3, 4], which is nothing but noticing that the ideal algorithm for the free Lagrangian above is to perform the simulation in Fourier space by adding the momentum dependent kinetic energy part

\[ H = \sum_p \frac{1}{\omega_p^2} \pi(p) \pi(-p) + \omega_p^2 \phi(p) \phi(-p). \] (5.4)

This \( p \)-dependent kinetic energy part will take into account exactly the frequency differences of the modes and, in fact, the \( p \)-dependence for the step size then drops out completely from the Hamilton equation of motion, as one can easily check. This hybrid algorithm is then equivalent to simulating \( V \) independent harmonic oscillators with frequency 1 in lattice units. However, nobody would be impressed if one can simulate a free theory effectively. When the interaction terms are added, doing the simulation completely in Fourier space is sometimes hopeless. This is particularly true if the interaction is of the \( \phi^4 \) type, which is completely local in real space, but highly nonlocal in Fourier space. Therefore, the hope is that we use a Fast Fourier Transformation program to go back and forth between the real space and the Fourier space. When the quadratic parts are evaluated, we go to the Fourier space, and when the interaction part is needed, we go to the real space. Obviously, this depends greatly on how fast one can do the Fourier transform. It turns out the existing FFT package runs reasonably well on the cray with a speed of \( 300 - 500 \) Mflop on the C90-machine. Another complication is that in the interacting theory we do not know what type of \( p \)-dependent kinetic energy term to add. The only clue is perturbation theory, however, one would expect that the low energy modes should be very well described by the renormalized parameters. It turns out that the main effect is the broadening effect due to \( M \), and \( M \) does not get renormalized very much. Therefore, putting in the bare value for \( M \) basically overcomes most of the critical
slowing down. We are able to perform the simulation with an autocorrelation time which is below 10 hybrid Monte Carlo trajectories with each trajectory consisting of 15 – 20 steps. Although this performance is not ideal, it works thousands of times better than the old programs, for which the autocorrelation time was hopelessly long. Also, in the Fourier accelerated Hybrid Monte Carlo, it is trivial to extend the algorithm to the improved actions. Since the quadratic part is evaluated in the Fourier space, it does not cost anything more for us to use the improved propagator as compared with the naive one. If this were implemented in the real space, it would require a lot more work.

All of our results were obtained with the appropriate Fourier accelerated Hybrid Monte Carlo program. We currently have only the version for the finite bare coupling constant. Therefore, all results presented here are for some finite bare coupling constant. However, some of our simulation points have a rather large bare coupling constant in continuum notation, therefore, we expect that most of the physically interesting results will be quite similar in the nonlinear limit.

5.2 The Extraction of Physical Parameters

We will now extract some physical quantities from our simulation results [6]. One of the most interesting quantities is the vacuum expectation value \( v \). This is the quantity which sets the energy scale of the simulation. In the old simulations, this parameter was obtained by measuring the bare expectation value of the averaged field variable. The wave function renormalization constant was then obtained from a linear fit to the momentum space propagator. From these quantities, the renormalized vev is then obtained using

\[
v_R = Z^{-1/2}v_0. \tag{5.5}
\]
The crucial point is the measurement of the wave function renormalization constant. But in our case, things are more complicated. The momentum space propagator will not only contain the usual $p^2$ term, but will also contain the higher derivative terms. In general, the interaction will generate more terms which were not in the bare free propagator. This makes it more difficult for us to get a very accurate determination of the wave function renormalization constant.

Another way of extracting the renormalized vev is from the rotator correlation functions. Using the theory discussed in Chapter (4), we can write down an expression for the rotator correlation function $n^a(0)n^a(\tau)$, where $n^a(\tau)$ is the unit vector of the zeromode at a given time slice $\tau$

$$\langle n^a(\tau)n^a(0)\rangle = A \sum_l l(l+1)e^{-\beta\omega_r(l(l+1)-1/2)} \cosh[(2l+1)(\tau - \beta/2)\omega_r], \quad (5.6)$$

where $\omega_r = (2L^3v_r^2)^{-1}$ is the rotator energy unit. This correlation function is dominated by the rotator energy spectrum in the finite volume. All the other energy excitations are much higher than the rotator energy scale. Usually the lowest one is the one Higgs contamination, whose energy scale is an order of magnitude higher. This correction can be easily taken into account according to the formula given in Chapter (4). Since the rotator energy depends only on the renormalized vacuum expectation value (and the 3 volume), this is a direct way of extracting the vev. In our simulations, we have tried both methods and have obtained compatible results.

In Figure (5.1), a typical rotator correlation function is shown compared with the fit to the theoretical form. The bare parameters are shown at the top of the figure. The lattice size for this run is $16^3 \times 40$. The output data has a total statistic of 32k hybrid Monte Carlo trajectories. At very short distances, higher energy excitations will contribute. Therefore, the fit was performed from $\tau = 6$ all the way to the end. The fit is very stable if the starting point is after $\tau = 5$. The fit
Figure 5.1: The rotator correlation function is shown together with the theoretical fit. The fit starts at $\tau = 6$ and the quality of the fit is good. The disagreement of the theoretical curve with the data for small values of $\tau$ is because of the high energy contaminations.

is also very stable with respect to the number of rotator states ($n_{\text{max}}$ in the figure) that has been included. It turns out that any number which is greater than 3 would be adequate. In this fit, the correction of the single Higgs state is included using the formula described in Chapter (4). This correction is about 10 percent even at large $\tau$ values. This is because of the small vev value of our simulation. The corrections due to the other states are all very small at large $\tau$ values. It is clear that we have found a very good agreement with the theoretical formula.

For comparison, the momentum space Higgs propagator is shown in Figure (5.2). This momentum propagator was obtained from a run of the same input bare parameters as in Figure (5.1) except that it was on a cubic geometry of $16^4$
Figure 5.2: The momentum space Higgs propagator is plotted as a function of the lattice momentum squared for the bare parameters shown at the top. The solid curve is a fit of the data to the polynomial form up to order $\hat{p}^6$. The upper window is a magnified portion of the lower window in the range $\hat{p}^2 < 4$. The quality of the fit is reasonable, however, due to the ambiguity of the fitting functional form, the error in the fitted wave function renormalization constant $Z$ is rather large.

with the statistic of 20k trajectories. The form of the fitting function is taken to be $f(p^2) = Z^{-1} \hat{p}^2 + Z^{-1} m^2 + p_2 \hat{p}^4 + p_3 \hat{p}^6$. Note that the size of the coefficient of $\hat{p}^4$ term is quite significant which is a signal of strong interaction effects. We should keep in mind that the above function has no justification if the interaction is strong. In general, the interaction could introduce complicated functional forms to the full Higgs propagator. It could generate log $\hat{p}^2$ terms, higher polynomial terms and even terms that cannot be written as functions of $\hat{p}$ alone. Therefore, the size of the interaction terms like $\hat{p}^4$ basically reflects the ambiguity of the fit. If we had tried the same fit
but setting the coefficients of $\hat{p}^4$ to zero, we would have arrived at a rather different value of $Z$ ($Z^{-1} = 1.33$). From this we conclude that, due to the strong interaction, it would be very difficult to extract the wave function renormalization constant from the momentum space propagator. Other methods are needed for the extraction of the physical parameters and the momentum space propagator can only be used as an independent check.

Another important quantity is the mass of the Higgs particle. In the old simulations, there were also two ways of obtaining the Higgs mass. One way is to use a fit to the momentum space propagator. The mass obtained this way has both advantages and disadvantages. The advantage is that the signal is very clean and we get a very stable fit for the mass even with low statistics. We can fit the very low momentum portion of the momentum space propagator where the effects of the interaction terms are small and the mass values are rather stable. The disadvantage is that the mass obtained from the propagator is not yet the physical Higgs mass. We must use perturbation theory to relate the two masses. This is legitimate in the old $O(4)$ calculation because, in that case, the theory is perturbative and the perturbative formula offers us a rather accurate prediction. In a truly nonperturbative theory, however, this could be misleading. The mass obtained from the propagator fit, what we call the off-shell mass, could deviate significantly from the physical mass.

Another way of determining the Higgs mass is from the time slice correlation function of the Higgs field. In this approach, the lowest energy gap of the Higgs excitation is extracted and identified as the Higgs mass in the finite volume. This, of course, should be closer to the physical mass than the off-shell mass and, in a strongly interacting theory this is the only way to get a good control of the Higgs mass. In our simulation of the higher derivative theory, the interaction is much stronger than the conventional $O(4)$ case, therefore, we used this method to extract
the Higgs mass. The off shell Higgs mass was also determined and only served as a comparison.

\[ \kappa = 0.056 \quad M = 0.8 \quad \lambda = 0.4 \]

\[ m = 0.4021 \]

**Figure 5.3:** The time sliced Higgs propagator is plotted as a function of the Euclidean time separation \( \tau \) for the bare parameters shown at the top. The solid curve is a fit of the data to the single Higgs excitation. The fit was done in the range \( 5 < \tau < 17 \) to ensure that the higher energy excitations have died out. The quality of the fit is reasonable, but the error for the mass parameter remains to be determined.

In Figure (5.3), we have shown the time sliced Higgs correlation function as a function of the Euclidean time separation \( \tau \). The bare parameters are also shown at the top of the figure. At small distances, all higher energy excitations contribute, including the ghost states. Therefore, to ensure that we extract the lowest radial excitation, we started the fit from some \( \tau \) values so that the fit was stable from there.
on. The functional form that we used is the standard hyperbolic cosine function for a single excitation. The data of the correlation function is derived from a blocking analysis of 32k hybrid Monte Carlo trajectories. If we compare this fitted mass value with the off shell mass, we find that the difference is very significant, which means the interaction is really much stronger when compared with the conventional $O(4)$ case. The data points of the correlation function are highly correlated. Therefore, we should develop a method to determine the error of the fitted mass value.

To determine the error of the mass parameter, we performed the following blocking procedure. The output data is originally divided into small blocks. For this particular example, we had 80 blocks available. Due the large fluctuation, a single block is not enough to give stable mass values. Therefore, the small blocks are first grouped together to form $N_b$ larger blocks, large enough so that we can extract stable mass values from them. For each large block $i$, the following ratio is formed
\begin{equation}
R_i(\tau) \equiv \frac{G_i(\tau + 1) - G_i(\tau)}{G_i(\tau) - G_i(\tau - 1)},
\end{equation}
where $i$ runs from 1 to the total number of large blocks $N_b$. If we have only a single excitation that dominates the correlation function, then the correlation function should be of the form
\[G^{\text{theo}}(\tau) = A \cosh[m(\tau - L_t/2)] + B.\] (5.8)
Therefore, the ratio should only depend on the mass $m$ and the Euclidean time separation $\tau$,
\begin{equation}
R^{\text{theo}}(\tau) = \frac{\cosh[m(\tau + 1 - L_t/2)] - \cosh[m(\tau - L_t/2)]}{\cosh[m(\tau - L_t/2)] - \cosh[m(\tau - 1 - L_t/2)]},
\end{equation}
(5.9)
Then the blocked values $R_i(\tau)$ are set to the theoretical value and we can solve for the mass numerically for each $\tau$. The outcome of this procedure is called the “effective
mass”, denoted as \( m^i_{\text{eff}}(\tau) \). Then, the averaged effective mass is obtained by

\[
m_{\text{eff}}(\tau) = \frac{1}{N_b} \sum_{i=1}^{N_b} m^i_{\text{eff}}(\tau).
\] (5.10)

We can also obtain an error for the effective mass by

\[
\Delta m_{\text{eff}}(\tau) = \sqrt{\frac{1}{N_b(N_b - 1)} \sum_{i=1}^{N_b} [m^i_{\text{eff}}(\tau) - m_{\text{eff}}(\tau)]^2}.
\] (5.11)

We can then plot the effective mass as a function of the time separation \( \tau \), together with

\[\kappa = 0.056, \ M = 0.8, \ \lambda = 0.4\]

\[m_H = 0.402365, \ N_b = 5\]

![Figure 5.4: The effective mass plot for the time slice Higgs correlation function for the bare parameters listed at the top. The Higgs mass value is obtained from the \( \chi^2 \) fit to the plateau starting at \( \tau = 7 \). The dashed line tick marks denote the range of the fit. The horizontal solid line is the fitted mass value which is also labeled in the figure. The horizontal dashed lines denotes the error of the fitted mass value. The mass value from the effective mass plot is consistent with the value from the exponential fit.](image)

Figure 5.4: The effective mass plot for the time slice Higgs correlation function for the bare parameters listed at the top. The Higgs mass value is obtained from the \( \chi^2 \) fit to the plateau starting at \( \tau = 7 \). The dashed line tick marks denote the range of the fit. The horizontal solid line is the fitted mass value which is also labeled in the figure. The horizontal dashed lines denotes the error of the fitted mass value. The mass value from the effective mass plot is consistent with the value from the exponential fit.
with the appropriate errors. This is shown in Figure (5.4). We found that, since many states contribute for small values of \( \tau \), the effective mass is varying with \( \tau \). However, if we go to \( \tau \) values that are large enough, all the higher energy excitations die out exponentially and the lowest energy excitation dominates. Therefore starting from some \( \tau \) value, we should see a plateau behavior of the effective mass. The value of the plateau should basically be the energy of the lowest energy excitation. Since the signal is getting exponentially small with \( \tau \), the error of the effective mass function will grow significantly with \( \tau \). Usually near the endpoint \((\tau = L_t/2)\), the errors become so large that effective mass value is no longer meaningful. We can then perform a \( \chi^2 \) fit to the effective mass, giving higher weight to the more accurate points. From this fit, we can determine the mass and its error.

But this is not the whole story yet. In fact even in the second approach, what we extract is not the infinite volume Higgs mass. The reason for this is very simple. All the simulations are done in a finite volume, and finite size effects must be taken into account. Among all the finite effects, there is one effect that is most disturbing. In the infinite volume, the Goldstone particles are exactly massless. Therefore, the Higgs particle can decay into two Goldstone particles, thus the Higgs has a finite lifetime. In the simulation, however, because the volume is finite, the lowest Goldstone pair is not at zero energy, but is equal to \( 4\pi/L \). This number is rather large for most of our simulations. In fact, it is larger than the Higgs mass itself. So the situation that we have in our simulation is that the Higgs is lighter than the Goldstone pair, and it therefore cannot decay. Of course, when the volume is increased, the Higgs mass energy level will meet the two Goldstone levels and the so-called level crossing phenomenon occurs. This was noticed quite some time ago. In fact, many groups have used this picture to get both the physical Higgs mass and its width from the measurement of the two Goldstone levels. In this picture, the Higgs
is viewed as a resonance of the Goldstone Goldstone scattering process. Lüscher derived a formula which relates the Goldstone pair energy level in the finite volume to the infinite volume Goldstone-Goldstone scattering phase shift. By measuring the two Goldstone energy levels as accurately as possible for various volumes, one gets the continuum scattering phase shift profile in an energy range. If all the parameters are well chosen, one would be able to see a phase shift stepping from almost zero to almost $\pi$ exactly at the threshold energy which is equal to the physical Higgs mass. One would also be able to get the physical width of the Higgs by fitting it to the Breit-Wigner shape near the resonance. So, instead of fighting against the finite volume effects, one could utilize it to gain precious information about the continuum theory.

To carry out a similar calculation in our model is more difficult than the usual $O(N)$ model. First of all, we must establish an equivalent formula in the higher derivative theory which can relate the energy levels in the finite volume to the phase shift in the infinite volume. Secondly, we have extra particles in our model, namely the ghost pairs. We have to control their contribution to the correlation functions in order to get reliable results for the two Goldstone energy levels. Thirdly, our model requires much more computing power to get good stable results for the time sliced correlation functions. The detailed analysis of this problem is given in the next chapter.

The simulation results we have obtained belong to one of the following two categories. One is performed with the naive discretization action and the other category is performed by using the improved action. We have done simulations in both phases of the theory. The following table summarizes the bare parameter and extracted physical quantities of the points. In this table, points $A$ through $G$ are the results for the naive action while points $H$ through $J$ are for the improved action.
Point $G$ and point $J$ are in the symmetric phase, while all other points are in the broken phase.

In the symmetric phase, the important physical quantity is the renormalized coupling constant, which could be defined to be the connected 4-point function at zero external momenta. In order to get this quantity, the propagator mass is measured. The renormalized coupling constant is directly measured by forming the connected 4-point function. The measurement of the renormalized coupling constant is very noisy, which requires large statistics of the data. We used the following formula to extract the connected four point function

$$\lambda_R = \frac{\Omega m_R^4}{24} \left( \frac{3N}{N+2} \right) \left( \frac{\langle \bar{\phi}^2 \rangle^2}{\langle \bar{\phi}^2 \rangle^2 - \langle \bar{\phi}^4 \rangle} \right),$$

(5.12)

where $N$ is the number of components of the field, $m_R$ is the propagator mass and
\( \Omega \) is the 4-volume of the system. The quantity \( \bar{\phi}^2 \) is defined to be \( \sum_{a=1}^{N} \bar{\phi}^a \bar{\phi}^a \) where \( \bar{\phi}^a \) is the 4-volume average of the field \( \phi^a(x) \). The quantity \( \bar{\phi}^4 \) is just a short hand notation for \((\bar{\phi}^2)^2\), and the bracket means the Monte Carlo ensemble average. It is the subtraction in the bracket which causes most of the noise. Therefore, in order to get sensible results we have accumulated large statistics for the two points in the symmetric phase (Point G and J in the table). In Figure (5.5), we have shown the

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure5_5.png}
\caption{The renormalized coupling constant (connected four point function at zero external momenta) is plotted for individual runs. Due to the subtraction the signal is quite noisy and a large statistic is needed to get a sensible accuracy for this quantity.}
\end{figure}

renormalized coupling constant for individual runs for the higher derivative \( O(4) \) model. It can be seen that the result is quite noisy and the points scatter a lot around the average. Usually 100\( K \) is needed for an error of about 10 percent.
We can now compare the renormalized coupling constant that we measured for the higher derivative $O(4)$ model with that of the conventional $O(4)$ model [7]. In the symmetric phase (point G and J), we found that the renormalized coupling constants were much larger than in the old lattice simulation results of $O(4)$ model. In the conventional $O(4)$ model, when the correlation length was about $2 - 3$ the renormalized coupling constant $\lambda_R$ was typically of the order of $0.6 - 0.8$. In our model, however, we saw a huge jump (about a factor of 2 to 3) of the renormalized coupling constant. This is a signal that the higher derivative model is much more strongly coupled than the conventional $O(4)$ model. Recall that, from the large $N$ calculations in Chapter (3), large $N$ also predicts a jump in the renormalized coupling constant in the symmetric phase. Therefore, our simulation results agree with the large $N$ results qualitatively.

In the broken phase, the renormalized vacuum expectation values are obtained using the rotator correlation functions as described above. The errors are estimated from a blocking analysis of the data.

The Higgs mass is taken to be lowest radial energy excitation in the finite volume. As described above, we tried two ways of extracting this energy gap. One by fitting the time sliced correlation function to the hyperbolic cosine function, the other from the effective mass plot. Both methods gave compatible results and the errors are determined from the $\chi^2$ fit of the effective mass plateau in the appropriate range.

Identifying this energy gap with the infinite volume Higgs mass is of course a rather crude approximation and is subject to finite volume corrections. However, as shown in the table, we did not see a significant change in the $m_H/v_R$ ratio when the lattice volume was increased. In fact, they are compatible with each other within errors. We also tested this within the framework of the large $N$ approximation.
We found that the ratio $E(L)/v(L)$ was rather stable when the size of the box was changed, as long as the box size was not too small and the energy crossing phenomenon had not occurred. And the value of the ratio was in agreement with the infinite volume large $N$ value. Therefore, we expect that this ratio represents the feature of the continuum higher derivative theory. The correct way of extracting the Higgs mass has to come from the finite volume resonance picture, which we will discuss in the next chapter.

Another issue in the Higgs mass bound problem is to determine how much scaling violations (cutoff effects) are present in our results. This turns out to be a rather subtle issue. To study this problem, we have to answer the following two questions: (1) what is the nature of the scaling violations in our model and, (2) how can we calculate the scaling violations once the Higgs mass and the ghost parameters are known.

First we will review how the above two questions are answered in the conventional $O(N)$ model simulations. In the conventional $O(N)$ model, the scaling violation is due to the hypercubic lattice that violates Euclidean (or rotational) invariance. This scaling violation can be defined both perturbatively and nonperturbatively. To calculate this scaling violation, we can check the rotational invariance of some quantity, for example, the free propagator of the field [12], or evaluate the Goldstone scattering amplitude and compare with perturbation theory [8, 9, 10, 11]. The second method seems to be more closely related to measurable quantities, but it relies on the perturbative nature of the problem. It worked out nicely for the conventional $O(4)$ simply because even at the highest bound, the theory is still perturbative. The first method offers us an unambiguous result without using perturbation theory.

Now, let us look at the situation for the higher derivative lattice theory. People tend to think that in the higher derivative $O(4)$ theory there exist two types
of scaling violations. One is the effect due to the lattice; the other one is what is usually called the Pauli-Villar cutoff (or ghost) effects. However, such a statement is very misleading. In fact, as we have shown in the previous chapters, this should not be the view, at least not the only view, of the higher derivative theory. This theory is a well defined field theory which has a unitary $S$-matrix and the ghost effects can easily evade the experimental tests. It is also a well-defined theory free of divergences. Therefore, if we could do the simulation in the continuum, we would have had no cutoff effects at all. It is only because the computer cannot handle infinite number of variables that we have to introduce the underline lattice to the theory. As long as we can constrain our lattice effects to be small, our simulation results should represent the higher derivative $O(4)$ model in the continuum. In other words, there are no “ghost effects” if the ghosts are well hidden from any experiment.

As stated previously, in analyzing the lattice effects, perturbation theory should only be taken as a hint. There have been ways of doing nonperturbative analysis of the lattice effects, though none of them is really sophisticated. One of the things that could be done is to analyze the breaking of the Euclidean invariance of the free propagator at some given parameters. This was first discussed by Lang et. al. in 1988 [12]. Although it only uses the tree level propagator, it is still a very good measurement of the amount of lattice violations in the theory. Obviously, going beyond this using perturbation theory is hopeless if the theory is strongly interacting. One can try to carry out the same analysis for the propagator in the large $N$ approximation, but again, the justification for the large $N$ approximation at $N = 4$ is not very promising either.

Let us now review some of the basic ideas of how this procedure is carried out for the propagator. On the lattice, the propagator in momentum space is, in general, a function of every individual momentum component. In the contin-
uum, however, it should only depend on the combination $p^2 = \sum_{\mu=1}^{4} p_\mu p_\mu$ due to Euclidean invariance. This symmetry is violated on the lattice and we can define a quantity $\mathcal{N}_G$ which represents the amount of violation due to the lattice. For the inverse momentum space propagator, the quantity $\mathcal{N}_G$ is defined in the following way. Let us pick some prescribed momentum scale $p_{cut}$ in lattice units, and pick our reference momentum to be $p_0 = (p_{cut}, 0, 0, 0)$. Then we can form all the momenta that have the same magnitude as this reference momentum in the form $\mathcal{R}p_0 = p_{cut}(\cos \theta_1, \sin \theta_1 \cos \theta_2, \cos \theta_1 \sin \theta_2 \cos \theta_3, \cos \theta_1 \sin \theta_2 \sin \theta_3)$. We can then define the rotational invariance violation by $\mathcal{N}_G$ by

$$\mathcal{N}_G(p_{cut}) = \int d\mathcal{R} \sqrt{\frac{(G(\mathcal{R}p_0) - G(p_0))^2}{G(p_0)^2}},$$

where $d\mathcal{R}$ is the invariant measure for the rotational group normalize in such a way that $\int d\mathcal{R} = 1$. Obviously this quantity is identically zero in the continuum where the rotational invariance is restored. On the lattice, the size of this quantity is a measure of the lattice effects in the discretized theory. In principle we can define similar quantities for other functions.

We have performed the rotation invariance analysis for our simulation points using both the tree level and large $N$ approximation. In Figure (5.6), we have shown some of the rotational invariance violations for the tree level propagator of our simulation points. We found that all our simulation points have very small lattice effects. For example, even with the naive propagator, in the Higgs mass range where we did our simulation, the rotational invariance violation is not larger than the old $O(4)$ simulation points with correlation length of $2 - 3$.

We can also calculate the finite volume lattice violation in both the free propagator and in the large $N$ approximation. In a finite box with lattice structure the lattice momenta are discrete and can only be multiples of $2\pi/L$. For each integer
Figure 5.6: The rotational invariance violation for the free inverse propagator on an infinite hypercubic lattice is plotted for various cases. The bottom two curves are the naive propagator and the one using the improvement up to 14th order. The upper two boxes show the Pauli-Villars case for $M = 2$ (the solid lines) and $M = 0.8$ (the dashed lines) when using the naive and improved action. It is clearly seen that for the parameters that our simulation are performed, the rotational invariance violation is very small.

For $n_{\text{cut}}$ there will be more than one set of solution $(n^{(i)}_1, n^{(i)}_2, n^{(i)}_3, n^{(i)}_4)$ to the equation $n_{\text{cut}} = n^2_1 + n^2_2 + n^2_3 + n^2_4$. Denoting the total number of solutions by $D(n_{\text{cut}})$, we can then define the counterpart of $N_G$ in the finite lattice

$$G(n_{\text{cut}}) = \frac{1}{D(n_{\text{cut}})} \sum_{i=1}^{D(n_{\text{cut}})} G((\frac{2\pi}{L})n^{(i)}_1, (\frac{2\pi}{L})n^{(i)}_2, (\frac{2\pi}{L})n^{(i)}_3, (\frac{2\pi}{L})n^{(i)}_4),$$

$$N_G(n_{\text{cut}}) = \sqrt{\frac{1}{D(n_{\text{cut}})} \sum_{i=1}^{D(n_{\text{cut}})} \frac{G((\frac{2\pi}{L})n^{(i)}_1, (\frac{2\pi}{L})n^{(i)}_2, (\frac{2\pi}{L})n^{(i)}_3, (\frac{2\pi}{L})n^{(i)}_4) - G(n_{\text{cut}})^2}{G(n_{\text{cut}})^2}}.$$  

Due the finite size effects, the momentum lattice is coarse grained. This will result in some zigzag behavior of the function $N_G(n_{\text{cut}})$, as $n_{\text{cut}}$ is increasing. However, for
a reasonably large lattice, we will recover the infinite lattice results. In Figure (5.7),

![Diagram showing rotational invariance violation for large-N inverse propagator](image)

**Figure 5.7:** The rotational invariance violation for the large $N$ propagator is plotted for different lattice sizes. The bare parameters are chosen to be close to the ones in our simulation. For small lattices, because the momentum is discrete, the function is not smooth. But for the larger lattices the function approaches the infinite volume result.

this rotational violation is shown for one of our simulation points for the large $N$ propagator. All the rotational invariance violation are well under one percent level. We are therefore confident that our results should represent the features of the higher derivative theory in the continuum.
References

[1] A. D. Kennedy and B. Pendleton, Nucl. Phys. B (Proc. Suppl.) 20 (1991) 118.

[2] G. Parisi, Progress in gauge field theory, ed. G. ’t Hooft et al. (Plenum, New York, 1984) 531.

[3] G. Batrouni, G. Katz, A. Kronfeld, G. P. Lepage, P. Rossi, B. Svetitsky and K. Wilson, Phys. Rev. D32 (1985) 2736.

[4] E. Dagotto and J. B. Kogut, Nucl. Phys. B 290 (1987) 451.

[5] K. Jansen, J. Kuti, C. Liu Phys. Lett. B309 (1993) 127.

[6] C. Liu, K. Jansen and J. Kuti, Nucl. Phys. B 34 (Proc. Suppl.), (1994) 635.

[7] J. Kuti, L. Lin, Y. Shen, Nucl. Phys. (Proc. Suppl.) B 4 (1988) 397; Phys. Rev. Lett. 61 (1988) 678.

[8] M. Lüscher and P. Weisz, Phys. Lett. B212 (1988) 472.

[9] A. Hasenfratz et al., Nucl. Phys. B317 (1989) 81.

[10] M. Göckeler, H. Kastrup, T. Neuhaus and F. Zimmermann, Nucl. Phys. (Proc. Suppl.) B 26 (1992) 516.

[11] U. M. Heller, H. Neuberger and P. Vranas, Nucl. Phys. B405 (1993) 557.
[12] C. B. Lang, Phys. Lett. B229 (1989) 97; Nucl. Phys. B (Proc. Suppl.) 17 (1990) 665.
Chapter 6

Extracting Scattering Phase Shift Using Finite Size Techniques

6.1 Resonance in Finite Volume

In the previous chapter we argued that extracting the mass parameter of an unstable particle in a finite volume is not a trivial task. For the volume that people usually perform their Monte Carlo simulations, the lowest two Goldstone particle state has an energy eigenvalue which is higher than the Higgs mass parameter. This means that in such volumes the Higgs cannot decay into the Goldstone pair as it should in the infinite volume, even if the interaction between the Higgs and two Goldstone state is turned on. This problem can be solved in two ways if the theory is only weakly interacting. In the first conventional way, one tries to extract the propagator mass in the finite volume, then the finite volume corrections are added to get the propagator mass in the continuum infinite volume. After that the perturbation theory is used again to relate the propagator mass to the on-shell physical mass of the Higgs particle. The width of the Higgs can also be calculated using perturbation theory. This method heavily utilizes perturbation theory. The second method is to extract the infinite volume continuum results directly by measuring some quantity in the finite volume. With this method, one needs a general formula
which will relate the infinite volume quantities to the finite volume quantities without using perturbation theory. In the conventional $O(4)$ simulations both methods have been tried and they give compatible results. It is obvious that for our higher derivative $O(N)$ model, due to its strong interaction, only the second one can be used to analyze the finite size effects. In fact, the basic idea of the second approach is to make use of the finite size effects instead of fighting them. Let us now review some of the basic ideas of this approach.

We start with the conventional $O(N)$ model without the higher derivatives. The basic particle excitations in the broken phase in a finite box consist of Higgs excitations and Goldstone excitations. Consider the eigenstate of one Higgs excitation and the eigenstates of two Goldstone excitations. Due to the Euclidean invariance, 

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure6.1}
\caption{The zeroth order of the level crossing is shown schematically as a function of box size $L$. The Higgs excitation is $L$ independent while the two Goldstone excitations is decreasing with $L$. At some value of $L$, the Higgs energy level will cross the Goldstone energy levels and if the interaction between the two is turned on, the two levels will repel each other and split.}
\end{figure}
we can take the rest frame of the Higgs particle. There is a major difference between the energy of the Higgs excitation and the Goldstone excitations. The Goldstone pair with opposite three momenta has an energy eigenvalue which is dependent of the box size. The lowest one is $4\pi/L$ where $L$ is cubic box size. The Higgs excitation, however, will not depend on the box size and is just a constant. To the lowest order, these particles behave just like free particles. In Figure (6.1), the dependence of these eigenvalues are shown. After the interaction is turned on, the one Higgs excitation mixes with the Goldstone pair excitation. For small box sizes, when the Higgs mass is below the lowest Goldstone pair excitation energy for that box size, ordinary perturbation theory will give us the correction of these energy levels if the interaction is not too strong. For some larger box size, however, the Higgs excitation will cross the Goldstone pair excitation and for that particular box size, degenerate perturbation theory should be used to calculate the level crossing. If the interaction is weak, one would expect a plateau in a range of $L$ which should be identified as the physical Higgs mass and the splitting at the crossing point basically gives you the width of the Higgs particle. In order to use this picture of resonance in a finite box, a nonperturbative relation must be established from which one can get the relation between infinite volume quantities and the finite volume quantities. Finally, if the finite volume quantities are measured in the Monte Carlo simulations, we can use this relation to deduce the infinite volume results nonperturbatively.

6.2 Lüscher’s Formula

In the infinite volume, the Higgs particle is identified as a resonance in the isospin 0 channel in Goldstone-Goldstone scattering. As in any two particle scattering process, the scattering cross section is characterized by the scattering phase shift $\delta(E)$ at a given center of mass energy. When the center of mass energy is at the
physical Higgs mass, we see a peak in the scattering cross section and the scattering phase shift rises dramatically from almost zero to almost $\pi$. In this case, there is a resonance in the scattering process and a Higgs particle is produced. The mass of the Higgs particle is identified by the position of the peak or equivalently by the energy at which $\delta(E)$ crosses $\pi/2$. The width of the particle is given by the range in which $\delta(E)$ steps from almost 0 to almost $\pi$. For an ideal resonance, that is the resonance which is infinitely narrow, the scattering phase shift will step up exactly $\pi$. But for wide resonances the sharpness and the height of the step is greatly reduced. Therefore, the scattering phase shift in the infinite volume fully describes the properties of the Higgs particle.

People have derived a relation which relates the infinite volume phase shift to the two Goldstone particle energy eigenvalues in the finite volume. This relation, with the name Lüscher’s formula, was derived first by DeWitt in a different form [5]. Later Lüscher rederived it and expressed in a form suitable for nonperturbative Monte Carlo simulations [1, 2]. It was used by Zimmermann et. al. to study the conventional $O(4)$ model and proved to work very well [3, 4]. We now derive this formula with a method that is based on DeWitt, since this can be easily generalized to the higher derivative case.

Consider a quantum mechanical system governed by the Hamiltonian $H = H_0 + V$ in a three dimensional box whose side is $L$. We can define the resolvent operators $G(z)$ and $G^0(z)$ as

\[ G(z) = (z - H)^{-1}, \quad G^0(z) = (z - H_0)^{-1}, \]

\[ G(z) = G^0(z) + G^0(z)V G(z), \quad (6.1) \]

where $z$ is just an arbitrary complex number. Consider the matrix elements of
$G(z)$ between two states $|\alpha\rangle$ and $|\beta\rangle$. where $|\alpha\rangle$ and $|\beta\rangle$ are eigenstates of the free Hamiltonian $H_0$, i.e. $H_0|\alpha\rangle = E_\alpha|\alpha\rangle$, $H_0|\beta\rangle = E_\beta|\beta\rangle$. We have

$$\langle \alpha|G(z)|\beta \rangle = \frac{1}{z - E_\alpha} (\delta_{\alpha\beta} + \langle \alpha|VG(z)|\beta \rangle). \quad (6.2)$$

Let us now define the self energy operator such that

$$\langle \alpha|\Sigma(z)|\beta \rangle = \langle \alpha|VG(z)|\beta \rangle \langle \beta|G(z)|\beta \rangle. \quad (6.3)$$

Then the matrix element of $G(z)$ may be written as

$$\langle \alpha|G(z)|\beta \rangle = \frac{1}{z - E_\alpha} (\delta_{\alpha\beta} + \langle \alpha|\Sigma(z)|\beta \rangle (\beta|G(z)|\beta \rangle). \quad (6.4)$$

The self energy operator defined above satisfies the following integral equations

$$\langle \alpha|\Sigma(z)|\beta \rangle = \langle \alpha|V|\beta \rangle + \sum_{\gamma \neq \beta} \langle \alpha|V|\gamma \rangle \frac{1}{z - E_\gamma} \langle \gamma|\Sigma(z)|\beta \rangle. \quad (6.5)$$

Setting $\alpha = \beta$ in the above equation we get

$$\langle \alpha|G(z)|\beta \rangle = (z - E_\alpha - \langle \alpha|\Sigma(z)|\alpha \rangle)^{-1}. \quad (6.6)$$

Note that the pole of $G(z)$ in the complex $z$ plane should be the exact eigenvalue of state $|\alpha\rangle$, and we get

$$\epsilon_\alpha - E_\alpha = \langle \alpha|\Sigma(\epsilon_\alpha)|\alpha \rangle, \quad (6.7)$$

where $\epsilon_\alpha$ is the eigenvalue of the full Hamiltonian for the state that is perturbed from $|\alpha\rangle$. This formula tells us that the expectation value of the self energy operator in some state gives us the so-called energy shift which is the energy difference between the exact eigenvalues and the free eigenvalues.

Let us now look at this integral equation in a very large box, where the intermediate states are very dense and we would expect to be able to go to the
continuum limit. In fact, we can write down an expression

$$+ \sum \frac{|\gamma\rangle \langle\gamma|}{z - E_\gamma} = P \frac{1}{z - H_0} + \delta(z - H_0)\Phi(z), \quad (6.8)$$

where the function $\Phi(z)$ is given by the energy shell sum

$$\Phi(z) = \sum \frac{dE(z)}{z - E_\gamma}. \quad (6.9)$$

This relation is obtained in the following way. Imagine that $z$ is some real number and we take some small real positive number $\epsilon$ and divide the real axis into a small interval $(z - \epsilon, z + \epsilon)$ and the rest. For a very large box, the eigenvalues $E_\gamma$ will be very dense and they are treated separately, depending on whether they fall in the interval or not. For those states whose eigenvalues fall outside the small interval, the sum will better approximate the principal valued expression if we take smaller $\epsilon$ values. For any fixed $\epsilon$ there will be infinite eigenvalues which fall into the small interval, as long as the box size is going to infinity. For these states, if the operator is inserted in some smooth function of the energy, they are equivalent to the delta function which selects out the specific energy. The function $\Phi(z)$ is basically the degeneracy sum of all the states that has almost the same energy in the infinite volume.

With this relation we can rewrite Equation (6.4) in the following way

$$\langle\alpha|G(z)|\beta\rangle = \langle\alpha|V\rangle\beta\rangle + \sum_\gamma \langle\alpha|V\rangle\frac{|\gamma\rangle \langle\gamma|}{z - E_\gamma} \Sigma(z)|\beta\rangle - \langle\alpha|V\rangle\beta\rangle \frac{\langle\beta|\Sigma(z)|\beta\rangle}{z - E_\beta}. \quad (6.10)$$

If we now take $z = \epsilon_\beta$ and make use of Equation (6.7) we get

$$\langle\alpha|\Sigma(z)|\beta\rangle = \langle\alpha|(1 - VP\frac{1}{z - H_0})^{-1}V\delta(z - H_0)\Sigma(z)|\beta\rangle\Phi(z). \quad (6.11)$$

We can then multiply both sides by a factor of $2\pi\delta(E_\alpha - E_\beta)$. Note that the scattering
phase shift operator is given by
\[
\langle \alpha | - 2 \tan \delta | \beta \rangle = 2\pi \delta (E_\alpha - E_\beta) \langle \alpha | (1 - V P \frac{1}{E_\alpha - H_0})^{-1} V | \beta \rangle,
\] (6.12)
also we can take our states \( | \alpha \rangle \) to be diagonal in angular momentum, we then get
\[
\Phi_{\lambda\alpha}(\epsilon_\alpha) = -\pi \cot \lambda_\alpha(\epsilon_\alpha). \tag{6.13}
\]
This is the basic formula which relates the scattering phase shift in the infinite volume to the exact energy eigenvalues in the finite volume. To be specific with the function \( \Phi \), note that in the isospin 0 channel of two Goldstone particles with opposite momenta \( k \), we have the relation
\[
1 = \frac{L^3}{(2\pi)^3} \frac{(4\pi)k^2}{(4\pi^2) k E_1} = \frac{L^3}{4\pi^2} k E_1 dE,
\] (6.14)
where \( E_1 \) is the energy of one Goldstone particle. We get \( dE = 4\pi^2/(L^3 k E_1) \), so
\[
\Phi_0(z) = \sum \frac{2\pi^2}{L^3} \frac{1}{k E_1(z/2 - E_1(k))}
= \sum \frac{4\pi^2}{L^3} \frac{1}{k(k^2 - (\frac{2\pi}{L})^2 n^2)}
= -\frac{1}{\sqrt{\pi q}} Z_{00}(1, q^2), \tag{6.15}
\]
where we have used the dispersion relation for the Goldstone \( z/2 = k \) and \( q = kL/(2\pi) \). The zeta function is defined to be
\[
Z_{lm}(1, q^2) = \sum_n Y_{lm}(n), \tag{6.16}
\]
where the function \( Y_{lm}(n) \) is the usual spherical harmonics. When this expression is
substituted into the general formula, we get

$$\cot \delta_0(E) = \frac{1}{\pi^{3/2}q} Z_{00}(1, q^2),$$

$$E^2/4 = k^2 + m_\pi^2, \quad m_\pi = 0,$$

$$q = \frac{kL}{2\pi}.$$  \hspace{1cm} (6.17)

This is exactly Lüscher’s formula that has been used by Zimmermann et. al. in their simulation except that they were working with the nonzero mass case for the Goldstone particle. It is clear from the above derivation that the condition of the massive Goldstone is not necessary. In fact, as we will see below, we have tested the massless case in the conventional $O(4)$ case and got consistent results with Zimmermann et. al..

This problem can be understood in the following way. Recall that in Lüscher’s derivation of the formula, he assumes that the pion (Goldstone) has a finite mass due to the non-vanishing external source. This external source tilts the potential and makes the potential lower in the direction of the external source. Therefore in the potential valley it is not flat but rather has a slope. This is why the Goldstone particles become massive. Then the Higgs field is defined to be the 4-volume average of the field variable along that particular direction. The Goldstone field is defined to be the field along the directions that are orthogonal to the Higgs field. However, when the external source is gets smaller, the tilting in the potential becomes weaker. As a result, the fluctuation around the Higgs direction becomes stronger. In the limit of a vanishing external source, the special direction is not defined at all and the potential becomes totally $O(N)$ invariant. It is clear that in this limit, the Higgs field and the pion field is not well-defined. This is also seen in the finite volume
correction of the pion mass. Therefore, if the box is too small, we will not be able to
disentangle the energy correction to the one pion energy and the interaction between
the two. In this case, the correction to the single pion mass depends on the quantity
$m_\pi L$ exponentially. When the pion mass goes to zero, the finite size correction to
the single pion energy will be very large. This is the main reason that one has to
take the nonzero pion mass.

In fact, the situation in the $O(N)$ model is more subtle. First of all, the
massless pion dispersion relation is protected by the symmetry in the very large
volume limit. Therefore, the energy of a single pion would be exactly multiple of
$2\pi/L$, even if the interaction is turned on. Exactly at the vanishing external source,
we know that the above picture is not a good picture of the symmetry breaking
mechanism in the finite volume. Instead, we should use the Born-Oppenheimer
picture discussed in Chapter (4) . In the Born-Oppenheimer picture, the pions are
massless, and the zero momentum pion is replaced by the rotator excitations. The
Higgs field can also be meaningfully defined. As we have seen in Chapter (4) , there
will be no large finite volume corrections to the two pion energy hence the energy
shift in the finite box totally reflects the interaction between the two pions. Note
that there is no contradiction to the finite external source case. If the external
source is present and significantly different from 0, then the conventional picture of
the massive pion works very well and the Born-Oppenheimer picture would be a very
bad approximation since the potential is so tilted. On the other hand, the Born-
Oppenheimer picture is valid for very small external source where the conventional
picture breaks down. Therefore, our conclusion is that Lüsher’s formula will still
work even in the massless pion case, as long as the field definitions are adjusted
according to the Born-Oppenheimer picture described in detail in Chapter (4).
6.3 Integral Representation of the Zeta Function

In the Lüscher’s formula, the zeta function needs to be dealt with carefully. For the cubic geometry, it turns out that a useful integral representation of the function exists which we will now discuss [1].

In general, the zeta function is defined to be

\[
Z_{lm}(s, q^2) = \sum_{n \in \mathbb{Z}} \mathcal{Y}_{lm}(n)(n^2 - q^2)^{-s},
\] (6.18)

where the symbol \( \mathcal{Y}_{lm}(n) \) stands for the usual spherical harmonic functions and the summation is over all the three dimensional integers. In order to derive the integral representation, let us also define the heat kernel by

\[
K(t, x) = \frac{1}{(2\pi)^3} \sum_{n \in \mathbb{Z}} e^{i n \cdot x - t n^2}.
\] (6.19)

We will also need the truncated heat kernel

\[
K_{\lambda}^{lm}(t, x) = \frac{1}{(2\pi)^3} \sum_{|n| > \lambda} \mathcal{Y}_{lm}(n) e^{i n \cdot x - t n^2}.
\] (6.20)

Then the zeta function has the following representation

\[
Z_{lm}(s, q^2) = \sum_{|n| < \lambda} \mathcal{Y}_{lm}(n)(n^2 - q^2)^{-s} + \frac{(2\pi)^3}{\Gamma(s)} \int_0^\infty dt t^{s-1} e^{t q^2} K_{\lambda}^{lm}(t, 0),
\] (6.21)

as long as \( s \) satisfies the condition \( \text{Re}(s) > 1/2 + 3/2 \). Note that the combination
\( \exp(tq^2)K_{\lambda}^{\lambda}(t,0) \) has the following asymptotic behavior

\[
e^{tq^2}K_{\lambda}^{\lambda}(t,0) \sim e^{-t(\lambda^2 - q^2)}, \quad t \to +\infty,
\]

\[
e^{tq^2}K_{\lambda}^{\lambda}(t,0) \sim \frac{\delta_{l0}\delta_{m0}}{(4\pi)^2}t^{-3/2} + {\mathcal O}(t^{-1/2}), \quad t \to 0.
\]

(6.22)

Therefore we immediately have the following analytic continuation for the zeta function in the range \( Re(s) > 1/2, \)

\[
Z_{\lambda m}(s,q^2) = \sum_{|n|<\lambda} \mathcal{Y}_{\lambda m}(n^2 - q^2)^{-s} + \frac{(2\pi)^3}{\Gamma(s)} \left( \frac{\delta_{l0}\delta_{m0}}{(4\pi)^2(s - 3/2)} \right.
\]

\[
+ \int_0^1 dt t^{s-1} \left( e^{tq^2}K_{\lambda}^{\lambda}(t,0) - \frac{\delta_{l0}\delta_{m0}}{(4\pi)^2t^{-3/2}} \right)
\]

\[
+ \left. \int_1^{\infty} dt t^{s-1} e^{tq^2}K_{\lambda}^{\lambda}(t,0) \right).
\]

(6.23)

In particular for \( s = 1 \) we have

\[
Z_{\lambda m}(1,q^2) = \sum_{|n|<\lambda} \mathcal{Y}_{\lambda m}(n^2 - q^2)^{-1}
\]

\[
+ (2\pi)^3 \int_0^{\infty} dt \left( e^{tq^2}K_{\lambda}^{\lambda}(t,0) - \frac{\delta_{l0}\delta_{m0}}{(4\pi)^2t^{3/2}} \right).
\]

(6.24)

The above integral representation is suitable for numerical evaluation of the zeta function. The integrand is evaluated for any \( t \) value and the integrals are performed numerically using the standard integration subroutines (e.g. IMSL). When evaluating the integrand one has to distinguish the case for \( t > 1 \) and \( t < 1 \). The first line in the representation (6.19) is used for the case \( t > 1 \) while the second line is used for the case \( s < 1 \) for better convergence. It turns out that an accurate numerical answer can be obtained for \( q^2 \) values not larger than 10, which is the case in the
practical applications.

6.4 Simulation Results on the Conventional $O(4)$ Model

As mentioned in the previous section, we performed a test simulation first on the conventional $O(4)$ model without the external source term. Therefore, our pion dispersion is the massless dispersion. The simulation was done using a cluster update program which runs very efficiently on the alpha AXP workstation. In the simulation, we made measurements after every 10 cluster updates and for each lattice size a 100,000 to 200,000 measurements were accumulated. The operators that we took into account were the radial Higgs field, and the four lowest pion pair states. We chose our simulation point so that the Higgs mass would come out around $0.6$. We were also working in the nonlinear limit of the $O(4)$ model and the input bare parameter was the hopping parameter $\kappa$ which we fixed to be $0.315$. Old simulation results indicate that the Higgs mass for this point should be $m_H = 0.581$. We scanned the size of our 3-volume from 8 to 24 with a step of 2. The correlation functions were then analyzed to extract the energy levels in this isospin zero channel. The correlation matrix was diagonalized and the eigenvalues were used to extract the energy levels. The errors of the energy levels were obtained by blocking the data. These errors in the energy levels then translate into the errors in the phase shift when using Lüscher’s formula. The final results can be summarized in Figure (6.2), where we have plotted the the scattering phase shift as a function of the center of mass energy obtained from the application of Lüscher’s formula (the data points). The solid line is a perturbative fit to the data which yields a mass and width compatible with the expected results. The dashed line represent the perturbative results when the old values of $m_H$ are substituted in. The highest point is for the lattice size
Figure 6.2: The scattering phase shift is extracted using Lüscher’s formula in the isospin 0 channel with zero Goldstone mass. The solid line is the fit to the relativistic Breit-Wigner shape and the fitted values of Higgs mass and width are also shown. This is in good agreement with the perturbative prediction (dashed line).

$8^3 \times 32$ and this point overshoots the expected values. This could be because of the lattice effects and the subleading finite volume effects. The rest of the points agree nicely with the perturbative results. The large error bars for the larger lattices is purely due to the lack of the statistics. This plot is a clear indication that the formula also works in the massless case, as long as we define our Higgs field properly.
6.5 Lüscher’s Formula for Higher Derivative Theory

The relation in the higher derivative theory is quite similar to that in the conventional theory. We just have to repeat most parts of the previous derivation and make adjustments accordingly. In the case of the higher derivative theory, the Hamiltonian is still self adjoint, i.e.

\[ \eta H^\dagger \eta = H , \quad \eta H_0^\dagger \eta = H_0 . \] (6.25)

We will still define the resolvent operators as

\[ G(z) = (z - H)^{-1} , \quad G_0(z) = (z - H_0)^{-1} , \]

\[ G(z) = G_0(z) + G_0(z)H_1G(z) . \] (6.26)

We will set up the basis \(|\alpha\rangle\) such that

\[ H_0|\alpha\rangle = E_\alpha|\alpha\rangle , \quad \sum_\alpha |\alpha\rangle \langle \bar{\alpha} | \eta = 1 , \] (6.27)

where the eigenvalue \(E_\alpha\) could be complex. The state are chosen to satisfy \( \langle \bar{\beta} | \eta | \alpha \rangle = \delta_{\alpha \beta} \). We can now define the self energy operator according to

\[ \langle \bar{\alpha} | \eta \Sigma(z) | \beta \rangle = \frac{\langle \bar{\alpha} | \eta H_1 G(z) | \beta \rangle}{\langle \bar{\alpha} | \eta G(z) | \beta \rangle} , \] (6.28)

and it satisfies the following integral equation

\[ \langle \bar{\alpha} | \eta \Sigma(z) | \beta \rangle = \langle \bar{\alpha} | \eta H_1 | \beta \rangle + \sum_{\gamma \neq \beta} (z - E_\gamma)^{-1} \langle \bar{\alpha} | \eta H_1 | \gamma \rangle \langle \bar{\gamma} | \eta \Sigma(z) | \beta \rangle . \] (6.29)
Similarly the energy shift is given by the diagonal matrix element of the self energy operator.

\[ \Delta E_\alpha = \langle \bar{\alpha} | \eta \Sigma (E_\alpha + \Delta E_\alpha) | \alpha \rangle. \] (6.30)

In the large 3-volume limit, the intermediate state summation in the integral equation of the self energy reduce to the following

\[
\sum_\gamma \frac{|\gamma\rangle \langle \bar{\gamma}| \eta}{z - E_\gamma} = \sum_{\gamma, \gamma', \in \mathbb{R}} \frac{|\gamma\rangle \langle \bar{\gamma}| \eta}{z - E_\gamma} + \sum_{\gamma, \gamma' \not\in \mathbb{R}} \frac{|\gamma\rangle \langle \bar{\gamma}| \eta}{z - E_\gamma}
\]

\[
= \sum_{\gamma, |E_\gamma - z| < \epsilon} \frac{|\gamma\rangle \langle \bar{\gamma}| \eta}{z - E_\gamma} + \mathcal{P} \frac{1}{z - H_0}
\]

\[
= \delta(z - H_0) \Phi(z) + \mathcal{P} \frac{1}{z - H_0}. \] (6.31)

Taking \( z = E_\beta + \Delta E_\beta \) we again arrive at

\[ \langle \bar{\alpha} | \eta \Sigma(z) | \beta \rangle = \langle \bar{\alpha} | \eta (1 - H_1 \mathcal{P} \frac{1}{z - H_0})^{-1} H_1 \delta(z - H_0) \Sigma(z) | \beta \rangle \Phi(z). \] (6.32)

The delta function in the above equation restricts the intermediate states summation to take only the real energy eigenstates. The matrix element of the operator \((1 - H_1 \mathcal{P} \frac{1}{z - H_0})^{-1} H_1\) between the physical states is nothing but the phase shift as can be verified from the general formula established in Chapter (3). Therefore, we would conclude that the Lüscher’s formula will still work, even in the case of the higher derivative theory with ghost states.
6.6 Phase Shift for Higher Derivative Theory in $1/N$ Expansion

As we have established the validity for the Lüscher’s formula for the higher derivative, it is very instructive to show that this indeed will work out in the large $N$ expansion. Recall that the continuum scattering phase shift for the higher derivative theory has been calculated in Chapter (3) in the large $N$ expansion. There the unitarity is maintained in the large $N$ expansion and the phase shift could have

$$v=0.18 \quad M=5 \quad \lambda_0=720 \quad \theta=0.25\pi$$

![Graph showing the result of the scattering phase shift for the higher derivative theory in the large $N$ limit](image)

**Figure 6.3:** The result of the scattering phase shift for the higher derivative theory in the large $N$ limit is shown as a function of the center of mass energy. The data points are obtained from the two Goldstone particle energy eigenvalues in the finite cubic box in the large $N$ limit by applying Lüscher’s formula. The solid line is the continuum large $N$ calculation for the same set of parameters as described in Chapter (3). The corresponding cross section is also shown. The agreement of the two methods is clearly seen.
some microscopic acausal effects. To verify that Lüscher’s formula in the higher
derivative theory, we have evaluated the energy eigenvalues for the two Goldstone particle in the isospin 0 channel in the large $N$ limit. This is done by solving for the real roots of the matrix element $\langle h | (z^2 - H^2)^{-1} | h \rangle$. In the leading order of the $1/N$ expansion this matrix element reduces to the geometric summation of the Goldstone bubbles. Then these eigenvalues are substituted into Lüscher’s formula to extract the phase shift, which is then plotted against the center of mass energy of the scattering. In Figure (6.3), the result of this calculation is shown. The points are the phase shift values obtained from Lüscher’s formula. The solid line is the corresponding continuum calculation of the phase shift as described in Chapter (3). It is evident that the formula is working very well. We have tried the same procedure for other set of parameters and they all give good agreement with the continuum calculations.

### 6.7 Phase Shift Simulations for Higher Derivative Theory

The result from the large $N$ expansion makes us confident that the same procedure could be carried out for the higher derivative field theory just as it was done for the conventional $O(N)$ model. Owing to the improved action, we can now select our Higgs mass value to be around 0.7 and the ghost mass parameter at $M = 2.0$ and still keep the lattice effects small. This makes it possible to perform such simulations on the higher derivative $O(N)$ model. However, there are quite a number of technical difficulties.

One of the main difficulties is that some efficient algorithms that are available for the conventional theory break down miserably for the higher derivative theory. For example, the over relaxation algorithm is very slow for the higher derivative theory due to the neighbor gathering. The cluster algorithm is simply not working
at all (the whole lattice tends to become one huge cluster). In fact the only usable algorithm is the Fourier accelerated hybrid Monte Carlo algorithm, which only works for finite bare coupling. Also, it is not as efficient as the algorithms mentioned above for the conventional theory. This means that to really get the stable energy levels, we would have to run a rather long time.

Another difficulty is the understanding of the shape of the phase shift as a function of the center of mass energy. If the theory is strongly interacting, we can no longer hope to fit the simulation data to the perturbative results. A scheme to extract the physical parameters like the Higgs mass and its width is needed. If the Higgs resonance is well separated from the ghost, we could try the Breit-Wigner shape near the resonance, neglecting the effects of the ghosts.

The simulation of this project is still in progress and we hope to release the results in the near future.
References

[1] M. Lüscher, Nucl. Phys. B354 (1991) 531; Nucl. Phys. B364 (1991) 237.

[2] M. Lüscher, U. Wolff, Nucl. Phys. B339 (1990) 222.

[3] F. Zimmermann, J. Westphalen, M. Göckeler and H. A. Kastrup, Nucl. Phys. B (Proc. Suppl.) 30 (1993) 879.

[4] F. Zimmermann, J. Westphalen, M. Göckeler and H. A. Kastrup, Nucl. Phys. B (Proc. Suppl.) 34 (1994) 566.

[5] B. S. DeWitt, Phys. Rev. 103 (1956) 1565.
Chapter 7
Conclusions

Our project was first motivated by the study of the Higgs mass bound problem in a Pauli-Villars regulated theory [3, 4, 5]. This theory can be viewed as a limiting case of the higher derivative $O(N)$ scalar field theory. The study of the higher derivative theory goes beyond the scope of the Higgs mass bound problem.

The higher derivative $O(N)$ model that we have studied is obtained from the conventional $O(N)$ scalar field theory by adding higher derivative terms to the Higgs kinetic energy [1, 3, 4]. We have established the consistent quantization procedure of the higher derivative scalar field theory, and have shown this theory to be finite and unitary with possible violations of microscopic causality [2]. Therefore, the ghost states in the theory can easily evade experimental tests. We have also studied the model nonperturbatively in computer simulations by introducing an underlying lattice structure.

In the continuum, the higher derivative $O(N)$ model can be viewed as the Pauli-Villars regulated conventional $O(N)$ model in the small $m_H/M$ limit, where $m_H$ is the Higgs mass and the $M$ is the Pauli-Villars mass parameter. It can also be viewed as a finite, well-defined and unitary theory with ghost excitations. The continuum large $N$ study of our model shows that this theory can incorporate a heavy Higgs particle in the TeV range, with the ghost pair well hidden at a few
times heavier than the Higgs particle [3].

On the lattice, our model can represent different universality classes of models, depending on how the criticality is approached. It could represent the conventional trivial $O(N)$ model at criticality, in which case, the higher derivative terms indeed become irrelevant. However, in another limit, it could also represent the higher derivative $O(N)$ theory in the continuum, in which case, the theory is not trivial and the higher derivative terms cannot be viewed as irrelevant operators in the Lagrangian.

From our simulation results of the model, it is evident that any attempt to perform a systematic search of higher dimensional operators to determine the Higgs mass bound would not make any sense [5], since, as far as the Higgs mass bound is concerned, one cannot tell whether a higher dimensional operator is relevant for the problem or not.

In our nonperturbative simulation of the model, we find:

(1) Our model can generate a much heavier Higgs particle than the conventional $O(N)$ model, which is in agreement with the large $N$ result qualitatively. Without introducing the more complicated structures like technicolor, it is possible in our model to have a strongly interacting Higgs sector, which was excluded by earlier lattice studies of the conventional model.

(2) It is difficult to establish a bound for Higgs particle in our model, because by the time the Higgs is heavy enough, it would be impossible for us to define the scaling violations in our model. In fact, in our model, we believe the notion of the Higgs mass bound loses its meaning, unless some new nonperturbative definition is provided.

Many interesting theoretical issues remains unsolved for our higher derivative $O(N)$ model. For example, can this theory incorporate a techni-rho-like resonance
in the isospin 1 channel? This is obviously a nonperturbative problem. To answer it, we have to extract the phase shift in the isospin 1 channel for the higher derivative theory. We are still working on this issue.
References

[1] K. Jansen, J. Kuti, C. Liu Phys. Lett. B 309 (1993) 119.

[2] J. Kuti and C. Liu, to be published.

[3] K. Jansen, J. Kuti, C. Liu Phys. Lett. B309 (1993) 127.

[4] C. Liu, K. Jansen and J. Kuti, Nucl. Phys. B 34 (Proc. Suppl.), (1994) 635.

[5] U. M. Heller, H. Neuberger and P. Vranas, Nucl. Phys. B405 (1993) 557.
