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Hamiltonian Lattice Field Theory: Computer Calculations Using Variational Methods

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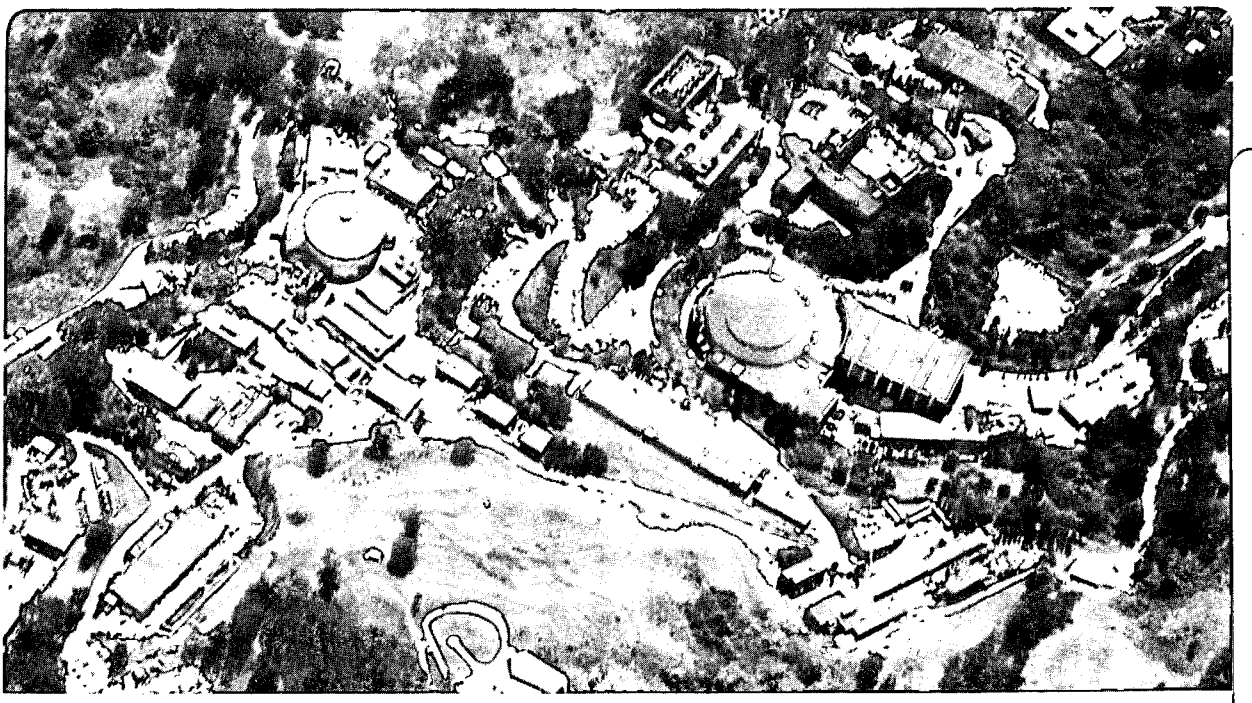

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Hamiltonian Lattice Field Theory: Computer Calculations Using Variational Methods *

Ph.D. Thesis

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Hamiltonian Lattice Field Theory: Computer Calculations Using Variational Methods

by

Robert Louis Zako

Abstract

I develop a variational method for systematic numerical computation of physical quantities—bound state energies and scattering amplitudes—in quantum field theory. An infinite-volume, continuum theory is approximated by a theory on a finite spatial lattice, which is amenable to numerical computation. I present an algorithm for computing approximate energy eigenvalues and eigenstates in the lattice theory and for bounding the resulting errors. I also show how to select basis states and choose variational parameters in order to minimize errors. The algorithm is based on the Rayleigh-Ritz principle and Kato's generalizations of Temple's formula. The algorithm could be adapted to systems such as atoms and molecules. I show how to compute Green's functions from energy eigenvalues and eigenstates in the lattice theory, and relate these to physical (renormalized) coupling constants, bound state energies and Green's functions. Thus one can compute approximate physical quantities in a lattice theory that approximates a quantum field theory with specified physical coupling constants. I discuss the errors in both approximations. In principle, the errors can be made arbitrarily small by increasing the size of the lattice, decreasing the lattice spacing and computing sufficiently long. Unfortunately, I do not understand the infinite-volume and continuum limits well enough to quantify errors due to the lattice approximation. Thus the method is currently incomplete. I apply the method to real scalar field theories using a Fock basis of free particle states. All needed quantities can be calculated efficiently with this basis. The generalization to more complicated theories is straightforward. I describe a computer implementation of the method and present numerical results for simple quantum mechanical systems.

To Mom and Dad,

whose endless love and support have enabled me to chase my dreams.

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Introduction

The Standard Model describes three of the four fundamental interactions—the electromagnetic, weak and strong—in terms of quantum gauge fields. It successfully explains phenomena with only electromagnetic and weak interactions, for which high-accuracy calculations of physical quantities are routinely performed using perturbation theory. For example, Kinoshita and Lundquist calculated the anomalous magnetic moment of the electron to within 2 parts in 10^7 [KL81]. But the Standard Model theory of strong interactions, quantum chromodynamics, is far less successful. Quantum chromodynamics does correctly predict many qualitative features of systems with strong interactions. But the problem is that no one has been able to calculate from quantum chromodynamics quantitative features of such systems at low, that is typical, energies. For example, no one has satisfactorily calculated the mass of the proton in terms of its constituent quarks.

Feynman remarked that "...the solution of the Yang-Mills theory with colored quarks [quantum chromodynamics] is a very, very important thing to achieve in a practical way with a reasonable accuracy." First, he stated, even though many people believe quantum chromodynamics is right, it would be good to be able to calculate its exact consequences. Second, if high-accuracy quantum chromodynamics calculations could be done and if small deviations were found between theoretical and experimental values, then the existence of a new quark, for example, might be discovered. Such an approach could be a practical alternative to building ever larger and more expensive particle accelerators. Third, he continued, if consequences of a theory like quantum chromodynamics could be calculated with reasonable accuracy, then the consequences of many proposed unified theories—such as $SU(5)$ and superstrings—could be calculated, allowing them to be ruled out or confirmed [Fey87].

Perturbation theory is useless for calculating in quantum chromodynamics at low energies because it yields a divergent asymptotic series in the effective coupling constant, which is of order one. The accuracy of a perturbation calculation actually decreases as additional terms are added. Unfortunately, in quantum chromodynamics the asymptotic series is not even Borel resummable, that is a correct finite result cannot be extracted from a knowledge of many terms in the divergent series ['tHo77].

Monte Carlo methods (lattice gauge theory) [Wil74] can, in principle, be used to calculate quantities in quantum chromodynamics to arbitrary accuracy. But, in practice, they have not been successful because the lattices obtainable with current computers are too small to give reasonably accurate results. Indeed, after eight years of fruitless research in lattice gauge theory, Wilson has abandoned the approach [Wil89].

Variational methods have been a standard technique in quantum chemistry for sixty years [Löw89, Wil89] and have been successfully applied to many atomic and molecular systems. For example, a simple pencil-and-paper calculation gives the ground state energy of the helium atom to within 2%. Kinoshita improved the result to within 4 parts in 10^7 using 39 terms [Kin57]. James and Coolidge accurately solved the hydrogen molecule [JC33]. More recently, Dunning [Dun89] and Partridge [Par89] have obtained reasonably accurate results for the first three rows of atoms (lithium–neon, sodium–argon, potassium–krypton) using variational techniques with only a few dozen gaussian basis states.

Variational methods were first applied to quantum field theory in the sixties by Schiff [Sch63] and Rosen [Ros68]. In the late sixties interest in variational methods declined because it was not known how to handle fermions nor how to extract physical information from variational quantum field theory calculations. In the early eighties the works of Barnes and Ghandour [BG80] and Stevenson [Ste84a, Ste84b, Ste85] on the gaussian effective potential renewed interest in variational methods, which were oftentimes combined with other techniques. Much of the subsequent research was presented in 1987 at the International Workshop on Variational Calculations in Quantum Field Theory [PP87]. In general, the application of variational methods to quantum field theory has been unsuccessful. Indeed, Feynman argued—more strongly than he believed—that the variational approach to quantum field theory is "no damn

good at all!" [Fey87]

Many researchers [Sch63, BG80, Ste85, Ing86, DHK87, Rit90] have worked in the continuum limit. This is problematic because the ground state energy is infinite, whereas excitations with respect to the ground state are finite. It is unclear what it means to minimize the infinite ground state energy. Moreover, quantum field theory in the continuum limit has an infinite number of dynamical variables, hence the Hilbert space of states is exceedingly large. As I argue in Section 1.4, it is overly optimistic to hope that the ground state can be modeled to any reasonable accuracy with only a finite number of parameters.

Other researchers [KDK86, Dun87] have worked with quantum field theory on a finite lattice. Typically, they have used fewer than 50 variational parameters. They have calculated the lowest few energies, identifying these—perhaps erroneously—as bound state energies. They have not quantified errors. And they have not adequately addressed the problem of renormalization, that is how to relate their bare coupling constants to physical coupling constants.

In general, physical results have been limited to the lowest few energies or to scaling behavior: The number of predicted quantities is barely more than the number of free parameters in the theory.[1]

In this paper I surmount many of the difficulties faced by previous researchers and develop a variational method for systematic numerical computation of physical quantities—bound state energies and scattering amplitudes—in quantum field theory. My aim is not to solve quantum chromodynamics, which is an exceedingly difficult task, but rather to develop a method that could, in principle, produce arbitrarily accurate results in such a theory, and to test the method in practice by applying it to simple theories of a single real scalar field. I also address the difficult issues of putting limits on errors and of optimizing the method to get a desired level of accuracy with a minimum amount of computation.

The main ingredients of my method are as follows: I use the hamiltonian formalism for quantum field theory; I use variational techniques; I choose free-particle states for a basis; I perform all calculations with a computer; I introduce a heuristic to

[1] The effective potential approach of Stevenson [Ste84a, Ste84b, Ste85] and others is promising, but here I do not pursue it.

minimize the error for a given level of computation; I calculate scattering amplitudes; and I establish a relation between bare and physical coupling constants. None of these ideas is particularly innovative, with the possible exceptions of my heuristic, my calculation of scattering amplitudes and my relating bare and physical coupling constants. But, to the best of my knowledge, this combination of ideas is new, and they form a promising approach to non-perturbative calculations in quantum field theory. The method is straightforward and has the added pedagogical benefit of presenting quantum field theory in a direct way.

The paper is organized as follows: In Chapter 1 I develop the method for an arbitrary quantum mechanical system. In Chapter 2 I introduce the theories to which I apply the method. In Chapter 3 I extend the method to quantum field theory. Finally, in Appendix A I describe a computer program implementing parts of the method and in Appendix B I presents preliminary results obtained using that program.

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Lastly, I give a big circle around the sun hug to Kayleen Hanna for her love and belief in me.

Life is a long road and graduate school but a brief crossing. I came to Berkeley seeking the important truths. Along the way I learned the questions were different than I had thought and found some partial answers. The important lessons did not come from a class room nor from a textbook, and I do not share them in this dissertation. But the road continues. I hope I will continue to learn and can share my discoveries with others.

Thanksgiving

Somehow I find myself far out of line from the ones I had drawn.
Wasn't the best of paths, you could atest to that... but I'm keeping on.

Would our paths if every great loss had turned out our gain?
Would our paths cross if the pain it had cost us was paid in vain?

There was no pot of gold, hardly a rainbow lighting my way.
But I will be true to the red, black and blues that colored those days.

I owe my soul to each fork in the road, each misleading sign,
'Cause even in solitude, no bitter attitude can dissolve my sweetest find.

Thanksgiving for every wrong move...
That made it right, that made it right.

— Adam Sultan, and the rest of Poidom
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Chapter 1

Variational Methods

In quantum theory a state of the system is described by a vector in a Hilbert space $\mathcal{V}$, and the system is described by a linear operator H, the hamiltonian, on $\mathcal{V}$ that is bounded below and hermitian ($H^\dagger = H$). An important problem is to find the energy eigenvalues $\epsilon_1, \epsilon_2, \ldots$ and corresponding energy eigenvectors $e_1, e_2, \ldots$ of H that satisfy the time-independent Schödinger equation:

$$H|e_k\rangle = \epsilon_k|e_k\rangle. \tag{1.1}$$

In general, it is difficult to find the eigenvalues and eigenvectors of H, since—even for simple quantum mechanical systems—$\mathcal{V}$ is infinite-dimensional.

In this chapter I develop a general variational method for calculating approximate eigenvalues and eigenvectors of a hermitian operator. In Section 1.1 I introduce the general method. In Section 1.2 I discuss the convergence of the method and describe how to estimate errors. In Section 1.3 I describe how the method can be optimized to minimize errors. Finally, in Section 1.4 I put the method in perspective and discuss the nature of variational methods.

1.1 Rayleigh-Ritz Method

In this section I introduce the Rayleigh-Ritz principle (1.26), which states that the eigenvalues of a hermitian operator restricted to a subspace are upper bounds

to the lowest eigenvalues of the operator. It is a practical way to find approximate eigenvalues and eigenvectors. I also introduce other related variational principles.

1.1.1 Rayleigh Variational Principle

My starting point is the more familiar Rayleigh variational principle. Let us label the eigenvalues of H in increasing order,

$$\varepsilon_1 \leq \varepsilon_2 \leq \cdots, \tag{1.2}$$

and choose the corresponding eigenvectors to be orthonormal,

$$\langle e_i | e_j \rangle = \delta_{ij}. \tag{1.3}$$

The *Rayleigh variational principle* characterizes the lowest eigenvalue ε_1 of H as the minimum value of $\langle H \rangle$,

$$\varepsilon_1 = \min_{v \in \mathcal{V}} \langle H \rangle_v, \tag{1.4}$$

and the corresponding eigenvector e_1 as a vector that minimizes $\langle H \rangle$. Here

$$\langle H \rangle_v = \frac{\langle v | H | v \rangle}{\langle v | v \rangle} \tag{1.5}$$

is called the *Rayleigh quotient* or, in physics language, the expectation value of H in the state v. We call v a *trial vector*. Here and in what follows we assume $v \neq 0$; otherwise $\langle H \rangle_v$ is undefined.

If H were bounded above instead of below, then another form of the Rayleigh variational principle would similarly characterize the highest eigenvalue ε_∞ of H as the maximum value of $\langle H \rangle$,

$$\varepsilon_\infty = \max_{v \in \mathcal{V}} \langle H \rangle_v, \tag{1.6}$$

and the corresponding eigenvector e_∞ as a vector that maximizes $\langle H \rangle$.[1]

[1] If the lowest eigenvalue is ℓ-fold degenerate, that is if $\varepsilon_1 = \cdots = \varepsilon_\ell$, then the corresponding eigenvectors $e_1, \ldots, e_\ell$ are not uniquely determined. In this case any $v = \theta_1 e_1 + \cdots + \theta_\ell e_\ell$ minimizes $\langle H \rangle$. Similarly if the highest eigenvalue is degenerate.

To demonstrate the Rayleigh variational principle, note that the eigenvectors of H form a complete orthonormal basis for $\mathcal{V}$,[2] thus a resolution of the identity operator on $\mathcal{V}$ is

$$1_{\mathcal{V}} = \sum_i |e_i\rangle\langle e_i|. \tag{1.7}$$

Since for any v in $\mathcal{V}$

$$\langle v | H | v \rangle = \sum_{ij} \langle v | e_i \rangle \langle e_i | H | e_j \rangle \langle e_j | v \rangle \tag{1.8a}$$

$$= \sum_i \varepsilon_i |\langle e_i | v \rangle|^2 \tag{1.8b}$$

$$\geq \varepsilon_1 \sum_i |\langle e_i | v \rangle|^2 \tag{1.8c}$$

$$= \varepsilon_1 \langle v | v \rangle, \tag{1.8d}$$

we conclude that

$$\min_{v \in \mathcal{V}} \frac{\langle v | H | v \rangle}{\langle v | v \rangle} \geq \varepsilon_1. \tag{1.9}$$

If we choose $v = e_1$, then

$$\min_{v \in \mathcal{V}} \frac{\langle v | H | v \rangle}{\langle v | v \rangle} \leq \frac{\langle e_1 | H | e_1 \rangle}{\langle e_1 | e_1 \rangle} = \varepsilon_1. \tag{1.10}$$

Hence the Rayleigh variational principle (1.4) follows. The form of the Rayleigh variational principle for the highest eigenvalue can be similarly demonstrated.

The Rayleigh variational principle states that any trial vector v provides an upper bound to ε_1:

$$\varepsilon_1 \leq \langle H \rangle_v. \tag{1.11}$$

In practice, one chooses an n-dimensional submanifold $\mathcal{W}$ of $\mathcal{V}$ parameterized by n parameters $\theta_1, \ldots, \theta_n$: $v = v(\theta_1, \ldots, \theta_n)$. Then the best upper bound within $\mathcal{W}$ is obtained by minimizing $\langle H \rangle$ with respect to $\theta_1, \ldots, \theta_n$. A better (or at least no worse) upper bound can be obtained by considering a larger submanifold, that is by considering additional variational parameters.

[2] Technically, this is only true if the spectrum of H is discrete. If the spectrum of H has a continuous part, then the corresponding eigenvectors are not in $\mathcal{V}$ since they have infinite norm. Such is the usual case, for example, with atomic hydrogen, which has a discrete spectrum of negative bound state energies and a continuous spectrum of positive unbound state energies. In what follows I will gloss over these mathematical subtleties and assume the spectrum of H is discrete.

1.1.2 Rayleigh Variational Principle Example

For example, consider the 1-dimensional anharmonic oscillator described by the hamiltonian

$$H = -\frac{1}{2}\frac{d^2}{dq^2} + \lambda_2 q^2 + \lambda_4 q^4 \tag{1.12}$$

in the configuration representation. Here I choose units such that $\hbar = m = 1$. Consider the trial vector

$$\psi(q) = e^{-\frac{1}{2}\omega q^2}, \tag{1.13}$$

where ω is a variational parameter. Then

$$\langle\psi|\psi\rangle = \int dq\, e^{-\omega q^2} = \sqrt{\frac{\pi}{\omega}} \tag{1.14}$$

and

$$\langle\psi|H|\psi\rangle = \int dq\, e^{-\frac{1}{2}\omega q^2}\left(-\frac{1}{2}\frac{d^2}{dq^2} + \lambda_2 q^2 + \lambda_4 q^4\right) e^{-\frac{1}{2}\omega q^2} \tag{1.15a}$$

$$= \sqrt{\frac{\pi}{\omega}}\left(\frac{1}{4}\omega + \frac{1}{2}\frac{\lambda_2}{\omega} + \frac{3}{4}\frac{\lambda_4}{\omega^2}\right). \tag{1.15b}$$

Thus

$$\langle H\rangle_\psi = \frac{1}{4}\omega + \frac{1}{2}\frac{\lambda_2}{\omega} + \frac{3}{4}\frac{\lambda_4}{\omega^2}. \tag{1.16}$$

The minimum of $\langle H\rangle$ occurs for ω satisfying

$$0 = \frac{d\langle H\rangle}{d\omega} = \frac{1}{4} - \frac{1}{2}\frac{\lambda_2}{\omega^2} - \frac{3}{2}\frac{\lambda_4}{\omega^3}. \tag{1.17}$$

If we choose $\lambda_2 = \frac{1}{2}$ and $\lambda_4 = 1$, then we find the minimum value of $\langle H\rangle$ is $\frac{13}{16}$ for $\omega = 2$. Thus $\varepsilon_1 \le 0.8125$, which should be compared to the exact value $\varepsilon_1 = 0.803\,770\,65\ldots$.

1.1.3 Minimax Principle

The Rayleigh variational principle provides upper bounds to the lowest eigenvalue ε_1, but what about higher eigenvalues? We can generalize the Rayleigh variational principle for the lowest eigenvalue, Equation (1.4), by restricting the trial vector v to be in the $(k-1)$-codimensional subspace of $\mathcal{V}$ orthogonal to $e_1, \ldots, e_{k-1}$:

$$\varepsilon_k = \min_{v \perp e_1, \ldots, e_{k-1}} \langle H\rangle_v. \tag{1.18}$$

The proof is essentially the same, noting that $\langle e_1|v\rangle = \cdots = \langle e_{k-1}|v\rangle = 0$. But this principle is not useful since it requires a knowledge of the *exact* lower eigenvectors $e_1, \ldots, e_{k-1}$, which, in general, we do not have.

A more fruitful approach is to generalize the Rayleigh variational principle for the highest eigenvalue, Equation (1.6), by restricting the trial vector v to be in the k-dimensional subspace of $\mathcal{V}$ spanned by $e_1, \ldots, e_k$:

$$\varepsilon_k = \max_{v \in \mathrm{sp}\{e_1, \ldots, e_k\}} \langle H\rangle_v. \tag{1.19}$$

Again the proof is essentially the same, noting that $\langle e_{k+1}|v\rangle = \langle e_{k+2}|v\rangle = \cdots = 0$. This principle is not directly useful either, since, in general, we do not know the *exact* eigenvectors $e_1, \ldots, e_k$.

But consider an arbitrary k-dimensional subspace $\mathcal{V}_k$ of $\mathcal{V}$. Since $\dim \mathcal{V}_k = k > k-1$, $\mathcal{V}_k$ must contain some vector v orthogonal to $e_1, \ldots, e_{k-1}$. Then $\langle e_1|v\rangle = \cdots = \langle e_{k-1}|v\rangle = 0$, hence $\langle H\rangle_v \ge \varepsilon_k$. Thus we conclude that

$$\max_{v \in \mathcal{V}_k} \langle H\rangle_v \ge \varepsilon_k. \tag{1.20}$$

Since this is true for an arbitrary k-dimensional subspace $\mathcal{V}_k$ of $\mathcal{V}$,

$$\min_{\mathcal{V}_k \subset \mathcal{V}} \max_{v \in \mathcal{V}_k} \langle H\rangle_v \ge \varepsilon_k. \tag{1.21}$$

But choosing $\mathcal{V}_k = \mathrm{sp}\{e_1, \ldots, e_k\}$, Equation (1.19) tells us

$$\min_{\mathcal{V}_k \subset \mathcal{V}} \max_{v \in \mathcal{V}_k} \langle H\rangle_v \le \max_{v \in \mathrm{sp}\{e_1, \ldots, e_k\}} \langle H\rangle_v = \varepsilon_k. \tag{1.22}$$

Thus we have demonstrated the *minimax principle*, sometimes called the *Poincaré principle*:

$$\varepsilon_k = \min_{\mathcal{V}_k \subset \mathcal{V}} \max_{v \in \mathcal{V}_k} \langle H\rangle_v. \tag{1.23}$$

The minimax principle is a generalization of the Rayleigh variational principle for the lowest eigenvalue, Equation (1.4). Since it characterizes eigenvalues without reference to exact eigenvectors, it does give a reasonable method for finding an upper bound to ε_k: One selects any k-dimensional subspace $\mathcal{V}_k$ of $\mathcal{V}$, and the maximum value of $\langle H\rangle$ on $\mathcal{V}_k$ is an upper bound to ε_k.

1.1.4 Rayleigh-Ritz Principle

The minimax principle is essentially the Rayleigh-Ritz principle. But the Rayleigh-Ritz principle replaces the computationally difficult problem of maximizing $\langle H\rangle$ on a k-dimensional subspace with the computationally easier problem of finding the k-th lowest eigenvalue of an operator on an n-dimensional subspace.[3] In particular, let $\mathcal{V}_n$ be an n-dimensional subspace of $\mathcal{V}$, $n \geq k$. Let P_n be the orthogonal projection operator from $\mathcal{V}$ onto $\mathcal{V}_n$. Note that P_n satisfies

$$P_n^2 = P_n, \quad P_n^\dagger = P_n, \quad \operatorname{tr} P_n = n. \tag{1.24}$$

The projection operator from $\mathcal{V}$ onto the orthogonal complement $\mathcal{V}_n^\perp$ of $\mathcal{V}$ is $P_n' = 1 - P_n$. In general, $\operatorname{tr} P_n'$ is infinite, that is P_n' projects onto the infinite-dimensional subspace $\mathcal{V}_n^\perp$. If $v \in \mathcal{V}_n$, then $P_n|v\rangle = |v\rangle$, but $P_n'|v\rangle = 0$. Similarly, if $v \perp \mathcal{V}_n$, then $P_n|v\rangle = 0$ but, $P_n'|v\rangle = |v\rangle$.

Now define

$$H_n = P_n H P_n. \tag{1.25}$$

Then H_n maps any v in $\mathcal{V}_n$ into $\mathcal{V}_n$, hence we can treat H_n as an operator on $\mathcal{V}_n$. Thus H_n has n eigenvalues $\varepsilon_1^{(n)} \leq \cdots \leq \varepsilon_n^{(n)}$ corresponding to n orthonormal eigenvectors $e_1^{(n)}, \ldots, e_n^{(n)}$ in $\mathcal{V}_n$. If v is orthogonal to $\mathcal{V}_n$, then $H_n|v\rangle = 0$. Thus any v orthogonal to $\mathcal{V}_n$ is an eigenvector of H_n with eigenvalue zero, but these are uninteresting. Think of H_n as an $n \times n$ submatrix of the, in general, infinite matrix H (Figure 1.1).

The *Rayleigh-Ritz principle* states that the eigenvalues $\varepsilon_1^{(n)} \leq \cdots \leq \varepsilon_n^{(n)}$ of H_n are upper bounds to the corresponding lowest n eigenvalues $\varepsilon_1 \leq \cdots \leq \varepsilon_n$ of H:

$$\varepsilon_k \leq \varepsilon_k^{(n)}, \quad k = 1, \ldots, n. \tag{1.26}$$

[3] In general, variational techniques are not computationally efficient for finding the *exact* eigenvalues and eigenvectors of a *finite* matrix: Other non-variational algorithms are almost always used. In particular, finding the minimum of a function on an n-dimensional space requires $O(n \log n)$ gradient evaluations. Evaluating the gradient of most functions related to H, including $\langle H\rangle$, requires at least $O(n^2)$ time. Thus finding the vector that minimizes $\langle H\rangle$, that is the eigenvector with the lowest eigenvalue, requires at least $O(n^3 \log n)$ time. In comparison, we can reduce an $n \times n$ hermitian submatrix of H to tridiagonal form using the Householder algorithm and then find *all* n eigenvalues and eigenvectors of the submatrix using the QL algorithm with implicit shifts, a computation that takes $O(n^3)$ time [PFTV88, Wil65]. Note that it takes $O(n^3)$ time to merely verify by direct multiplication that n alleged eigenvalues and eigenvectors are, indeed, such. Nonetheless, we are attempting to use variational techniques to find *approximate* eigenvalues and eigenvectors of an *infinite* matrix. There is no contradiction here, since the efficient numerical algorithms for finite matrices cannot be applied directly to infinite matrices.

This follows immediately from the minimax principle:

$$\begin{aligned}
\varepsilon_k &= \min_{\mathcal{V}_k \subset \mathcal{V}} \max_{v \in \mathcal{V}_k} \langle H\rangle_v && (1.27a)\\
&\leq \min_{\mathcal{V}_k \subset \mathcal{V}_n} \max_{v \in \mathcal{V}_k} \frac{\langle v|H|v\rangle}{\langle v|v\rangle} && (1.27b)\\
&= \min_{\mathcal{V}_k \subset \mathcal{V}_n} \max_{v \in \mathcal{V}_k} \frac{\langle v|P_n H P_n|v\rangle}{\langle v|v\rangle} && (1.27c)\\
&= \min_{\mathcal{V}_k \subset \mathcal{V}_n} \max_{v \in \mathcal{V}_k} \frac{\langle v|H_n|v\rangle}{\langle v|v\rangle} = \varepsilon_k^{(n)}. && (1.27d)
\end{aligned}$$

It is clear that we get better upper bounds by taking a larger subspace: If $k \leq n < n'$ and $\mathcal{V}_n \subset \mathcal{V}_{n'}$, then the minimax principle implies that

$$\varepsilon_k \leq \varepsilon_k^{(n')} \leq \varepsilon_k^{(n)}. \tag{1.28}$$

In practice, the Rayleigh-Ritz method is as follows: Choose a complete basis $\{u_i\}$ for $\mathcal{V}$, which for convenience we assume to be orthonormal:

$$\langle u_i|u_j\rangle = \delta_{ij}. \tag{1.29}$$

Then the projection operator P_n from $\mathcal{V}$ onto the n-dimensional subspace $\mathcal{V}_n$ spanned by the *selected basis states* $u_1, \ldots, u_n$ is

$$P_n = \sum_{i=1}^{n} |u_i\rangle\langle u_i| \tag{1.30}$$

and

$$H_n = \sum_{i,j=1}^{n} |u_i\rangle\langle u_i|H|u_j\rangle\langle u_j|. \tag{1.31}$$

Thus with respect to the $\{u_i\}$ basis H_n restricted to $\mathcal{V}_n$ is represented by the $n \times n$ matrix with elements $\langle u_i|H|u_j\rangle$ for $i, j = 1, \ldots, n$ (Figure 1.1). We can find the eigenvalues and eigenvectors of H_n by diagonalizing this matrix, a computation that takes $O(n^3)$ time [PFTV88, Wil65]. The n eigenvalues of H_n are upper bounds to the n lowest eigenvalues of H. Then we can redo the computation with a larger n to get better upper bounds.

	P_n	P'_n	
P_n	$H_n = P_n H P_n$	$P_n H P'_n$	selected basis states
P'_n	$P'_n H P_n$	$P'_n H P'_n$	unselected basis states

Figure 1.1: The hamiltonian H shown in block form relative to selected and unselected basis states.

1.1.5 Another Form of the Rayleigh-Ritz Principle

Unlike the Rayleigh variational principle, the minimax principle and the Rayleigh-Ritz principle refer explicitly to a finite-dimensional subspace of $\mathcal{V}$. If we want to approximate, say, ϵ_2, the Rayleigh-Ritz principle requires us to find the second lowest eigenvalue $\epsilon_2^{(n)}$ of H_n on some n-dimensional subspace $\mathcal{V}_n$. This calculation takes $O(n^3)$ time, which seems like a lot if n is 100 or 1000. Can we find upper bounds to eigenvalues other than the lowest without having to consider such large matrices? The answer is yes, but with a catch.

Suppose $e_1^{(k)}, \ldots, e_k^{(k)}$ are k vectors such that

$$\langle e_i^{(k)} | e_j^{(k)} \rangle = \langle e_i^{(k)} | H | e_j^{(k)} \rangle = 0 \quad \text{for } i \neq j, \tag{1.32}$$

that is are orthogonal with respect to both the usual inner product and the H inner product. Let us label the vectors such that $\epsilon_1^{(k)} \leq \cdots \leq \epsilon_k^{(k)}$, where

$$\epsilon_i^{(k)} = \langle H \rangle_{e_i^{(k)}}. \tag{1.33}$$

Then each $\epsilon_i^{(k)}$ is an upper bound to the corresponding eigenvalue ϵ_i of H:

$$\epsilon_i \leq \epsilon_i^{(k)}, \quad i = 1, \ldots, k. \tag{1.34}$$

This is simply a restatement of the Rayleigh-Ritz principle that does not refer explicitly to $\mathcal{V}_k$. The proof follows by choosing $\mathcal{V}_k = \mathrm{sp}\{e_1^{(k)}, \ldots, e_k^{(k)}\}$ and then showing that $e_1^{(k)}, \ldots, e_k^{(k)}$ are, in fact, eigenvectors of H_k.

It is easy to find vectors satisfying the orthogonality conditions (1.32) using a Gram-Schmidt process. Then $\epsilon_k^{(k)}$ is an upper bound to ϵ_k. We call $e_1^{(k)}, \ldots, e_{k-1}^{(k)}$

witness vectors, since they are required to verify that $\epsilon_k^{(k)}$ is an upper bound to ϵ_k. They "prop up" $\epsilon_k^{(k)}$ and prevent it from falling below ϵ_k. Thus if we can find k such vectors, we can put an upper bound on ϵ_k.

The catch is this: It is easy to find k such vectors but hard to find ones that give a strong upper bound to ϵ_k. We are reduced to rummaging through the, in general, infinite-dimensional $\mathcal{V}$ for a good $e_k^{(k)}$ (and witness vectors $e_1^{(k)}, \ldots, e_{k-1}^{(k)}$), which is like looking for a needle in a haystack. As Footnote 3 above indicated, it is computationally more efficient to diagonalize a linear operator on an n-dimensional space than it is to minimize a related function such as $\langle H \rangle$. We are better off using the standard Rayleigh-Ritz method.

I independently discovered this form of the Rayleigh-Ritz principle, although it is undoubtably known to other researchers.

1.1.6 Maximin Principle

Note that there is also a *maximin principle*:

$$\epsilon_k = \max_{\mathcal{V}_{k-1} \subset \mathcal{V}} \min_{v \perp \mathcal{V}_{k-1}} \langle H \rangle_v. \tag{1.35}$$

Its demonstration is similar to that for the minimax principle. It is a generalization of the Rayleigh variational principle for the highest eigenvalue, Equation (1.6). It is tempting to use the maximin principle to find lower bounds to eigenvalues. Unfortunately, doing so requires minimizing $\langle H \rangle$ over the, in general, infinite-dimensional subspace $\mathcal{V}_{k-1}^{\perp}$ orthogonal to some $(k-1)$-dimensional subspace $\mathcal{V}_{k-1}$, which is difficult to do.

1.1.7 History and References

The Rayleigh-Ritz method was discovered by Rayleigh [Ray45] and independently by Ritz [Rit08, Rit09]. Some researchers [Wei34, Löw65, DHK87] mistakenly state that the Rayleigh-Ritz method is practical for finding only the lowest eigenvalue, and incorrectly credit Hylleraas and Undheim [HU30] or MacDonald [Mac33] for the method applicable to any eigenvalue. My presentation above draws on Stak-

gold [Sta68], which in turn draws on the standard works by Mikhlin [Mik64] and Gould [Gou66]. Griffel [Gri81] is also a useful source.

1.2 Convergence and Error Estimation

We have seen that the Rayleigh-Ritz method gives approximations to the eigenvalues and eigenvectors of a hermitian operator. In this section I define the eigenvalue and eigenvector errors; I explain that the Rayleigh-Ritz method converges in the sense that errors can be made arbitrarily small by choosing the subspace dimension n to be sufficiently large; and I show how errors can be estimated.

1.2.1 Eigenvalue and Eigenvector Errors

I define the *eigenvalue error* η_k between an approximate eigenvalue $\overline{\epsilon_k}$ and the corresponding exact eigenvalue ϵ_k to be

$$\eta_k = |\overline{\epsilon_k} - \epsilon_k|. \tag{1.36}$$

When approximate eigenvalues are obtained with the Rayleigh-Ritz method, the absolute value is unnecessary since $\epsilon_k \leq \overline{\epsilon_k}$.

The definition of the eigenvector error is more complicated. Note that eigenvectors are not uniquely defined: If e_k is an eigenvector with eigenvalue ϵ_k, then so is θe_k for any $\theta \neq 0$. I assume any approximate eigenvector $\overline{e_k}$ is normalized to unity: $\langle \overline{e_k} | \overline{e_k} \rangle = 1$. Moreover, if the eigenvalue ϵ_k is ℓ-fold degenerate, that is if $\epsilon_k = \cdots = \epsilon_{k+\ell-1}$, then for any $\theta_1, \ldots, \theta_\ell$ not all zero $\theta_1 e_k + \cdots + \theta_\ell e_{k+\ell-1}$ is also an eigenvector with eigenvalue ϵ_k. Thus we are led to define the orthogonal projection operator Q_k onto the subspace of eigenvectors with eigenvalue ϵ_k. If ϵ_k is ℓ-fold degenerate, then Q_k projects onto an ℓ-dimensional subspace. In particular, I define

$$Q_k = \sum_{\{i:\epsilon_i=\epsilon_k\}} |e_i\rangle\langle e_i|. \tag{1.37}$$

I define the (squared) *eigenvector error* ζ_k between an approximate eigenvector $\overline{e_k}$ and the corresponding exact eigenvector(s) with eigenvalue ϵ_k to be the squared

norm of the part of $\overline{e_k}$ orthogonal to the space of eigenvectors with eigenvalue ϵ_k:

$$\zeta_k = \|(1 - Q_k)|\overline{e_k}\rangle\|^2 = 1 - |\langle e_k|\overline{e_k}\rangle|^2 - \cdots - |\langle e_{k+\ell-1}|\overline{e_k}\rangle|^2. \tag{1.38}$$

Recall that the norm $\|v\|$ of a vector v is $\langle v|v\rangle^{1/2}$.

1.2.2 Convergence of Eigenvalues and Eigenvectors

If the basis $\{u_i\}$ for $\mathcal{V}$ is complete, then we can make the eigenvalue error $\eta_k^{(n)}$ between $\epsilon_k^{(n)}$ and ϵ_k arbitrarily small by choosing the dimension n of the subspace $\mathcal{V}_n$ to be sufficiently large. That is for each k, $\epsilon_k^{(n)}$ converges to ϵ_k as $n \to \infty$ [Gri81, pp. 290–292], [Wei62, pp. 89–91]. On the other hand, if the basis $\{u_i\}$ is incomplete, that is if we exclude one or more basis vectors from the set, then, in general, $\epsilon_k^{(n)}$ converges to a value larger than ϵ_k as $n \to \infty$.

If the basis $\{u_i\}$ for $\mathcal{V}$ is complete, then we can make the eigenvector error $\zeta_k^{(n)}$ arbitrarily small by choosing n to be sufficiently large. That is for each k, $e_k^{(n)}$ converges to some eigenvector with eigenvalue ϵ_k, though not necessarily e_k, as $n \to \infty$ [Wei62, pp. 127–131].

Thus the Rayleigh-Ritz method is *systematic*: We can, in principle, calculate arbitrarily good approximations to eigenvalues and eigenvectors by choosing n to be sufficiently large.

In contrast, perturbation expansions usually do not provide arbitrary accuracy. In general, perturbation expansions are divergent asymptotic expansions in some coupling constant.[4] Typically, for a fixed coupling constant adding terms in a perturbation calculation increases the accuracy up to a point, but beyond that adding terms actually *decreases* the accuracy. For large coupling constants the most accurate perturbation calculation is often a 0th-order one, which is usually not very accurate at

[4]Suppose $H = H_0 + \xi H_{\text{pert}}$, where H_0 is a solvable unperturbed hamiltonian and ξH_{pert} is a perturbation depending on some parameter ξ. Then perturbation theory expresses any quantity f as a power series in ξ: $f(\xi) = f_0 + f_1\xi + f_2\xi^2 + \cdots$. The radius of convergence of the series is the distance to the singularity of $f(\xi)$ closest to the origin in the complex ξ-plane. Usually, H is a physical hamiltonian for positive ξ, but is unbounded below, hence unphysical, for small negative ξ. Thus $f(\xi)$ is poorly defined for small negative ξ, strongly suggesting that $f(\xi)$ has some kind of singularity at $\xi = 0$. In this case, the radius of convergence of the series is zero: The series is a divergent asymptotic expansion.

all.[5] This is probably the situation with quantum chromodynamics at low energies. In general, perturbation theory is *not* a systematic method for calculating physical quantities in quantum theory, in the sense that arbitrary accuracy is not obtainable.

1.2.3 Error Estimation

Although, in principle, we can achieve arbitrary accuracy by taking a sufficiently large n, in practice, the size of n we use is limited by the speed of current computer technology. Thus it is important to estimate the errors in our approximations. The usual approach is to use the Rayleigh-Ritz method to place upper bounds on eigenvalues and some other method to place lower bounds. One then lowers the upper bounds and raises the lower bounds until the desired accuracy is achieved.

I do not take this approach for a few reasons. First, note that lower bounds are intrinsically more difficult to calculate that upper bounds: We cannot find lower bounds by simply examining some restriction H_n of H to a finite-dimensional subspace $\mathcal{V}_n$ of $\mathcal{V}$. Since one can calculate numerical results only on a finite-dimensional subspace, one needs some additional crude information about H outside of $\mathcal{V}_n$ to find lower bounds [Wei62, p. 110].

For example, the *method of intermediate problems*, originally due to A. Weinstein and then modified by Aronszajn and later by Bazley and Fox, provides lower bounds to eigenvalues [Sta68, pp. 381–386], [Gou66]. But the method requires us to calculate the $n \times n$ matrix with elements $\langle u_i|V^{-1}|u_j\rangle$ for $i, j = 1, \ldots, n$. Here V is a positive-definite piece of H, and $u_1, u_2, \ldots$ are the known eigenvectors of $H_0 = H - V$. In general, computation of each matrix element requires numerical evaluation of an integral—a high-dimensional integral if we are working with quantum field theory

[5] Yamazaki [Yam84] uses a combination of variational and perturbative methods to calculate the eigenvalues of an anharmonic oscillator, my example in Section 1.1. His method shares many similarities with the one I present here. He uses a variational method to optimally separate out a piece H_0 of H, which describes a solvable harmonic oscillator. The separation depends in a complicated way on both the coupling constants λ_2, λ_4 and the eigenvalue number k. He then uses perturbation theory to find the corrections to the eigenvalues of H_0 due to $H_{\text{pert}} = H - H_0$. His method gives good results for all values of λ_2, λ_4 and k, at least up to 4th-order in perturbation theory. Nonetheless, I think his method still gives a divergent series: Beyond a certain point adding terms in his perturbation series actually decreases the accuracy. Thus his method is not, in principle, systematic. In practice, his method may be good enough, and it deserves further study, although here I do not pursue this direction.

on a finite but large lattice. Computational considerations discourage applying this method to quantum field theory.

Second and more importantly, whereas in quantum mechanics eigenvalues of H are physically significant, their meaning in quantum field theory is less clear. For example, the ground state energy has no physical significance and is conventionally set to zero. We will see in Chapter 3 that we need to approximate eigenvectors and matrix elements between eigenvectors, as well as eigenvalues, to calculate physical quantities in quantum field theory. Thus placing lower and upper bounds on eigenvalues is, by itself, of little use in quantum field theory.

Lastly, my emphasis is on developing a method for calculating physical quantities in quantum field theory. There are conceptual obstacles to doing so unrelated to the technical issues of how we find approximate eigenvalues and eigenvectors. In order to address these conceptual obstacles as quickly as possible, I sacrifice the rigor of the method of intermediate problems and similar methods for techniques that I can get to work.

In particular, my approach to errors follows that introduced by Temple [Tem28] and generalized by Kato [Kat49] and others (see references therein). Suppose we know H has at most one nondegenerate eigenvalue ε_k in the open interval $(\beta_{k-1}, \alpha_{k+1})$:

$$\varepsilon_{k-1} \le \beta_{k-1} < \varepsilon_k < \alpha_{k+1} \le \varepsilon_{k+1}. \tag{1.39}$$

In other words, β_{k-1} is a rough upper bound to ε_{k-1} and α_{k+1} is a rough lower bound to ε_{k+1}. Furthermore, suppose that for some vector $\overline{\varepsilon_k}$

$$(\Delta H)_k^2 < (\overline{\varepsilon_k} - \beta_{k-1})(\alpha_{k+1} - \overline{\varepsilon_k}), \tag{1.40}$$

where $\overline{\varepsilon_k} = \langle H \rangle_{\overline{\varepsilon_k}}$ and we define the *variance*

$$(\Delta H)^2 = \langle (H - \langle H \rangle)^2 \rangle = \langle H^2 \rangle - \langle H \rangle^2. \tag{1.41}$$

Then Kato proves the interval $(\beta_{k-1}, \alpha_{k+1})$ contains exactly one eigenvalue ε_k, which satisfies

$$\overline{\varepsilon_k} - \frac{(\Delta H)_k^2}{\alpha_{k+1} - \overline{\varepsilon_k}} = \alpha_k' \le \varepsilon_k \le \beta_k' = \overline{\varepsilon_k} + \frac{(\Delta H)_k^2}{\overline{\varepsilon_k} - \beta_{k-1}}. \tag{1.42}$$

Thus if we have a rough lower bound α_{k+1} to ε_{k+1} and a sufficiently good approximate eigenvector $\overline{\varepsilon_k}$, then we obtain a good lower bound α_k' to ε_k. Similarly, a rough upper

bound β_{k-1} to ϵ_{k-1} leads to a good upper bound β'_k to ϵ_k. Note that the condition (1.40) implies that $\beta_{k-1} < \alpha'_k$ and $\beta'_k < \alpha_{k+1}$.

Furthermore, the eigenvector error ζ_k between $\overline{\epsilon_k}$ and the eigenvector e_k with eigenvalue ϵ_k satisfies

$$\zeta_k \leq \frac{[\overline{\epsilon_k} - \frac{1}{2}(\beta_{k-1} + \alpha_{k+1})]^2 + (\Delta H)_k^2}{[\frac{1}{2}(\alpha_{k+1} - \beta_{k-1})]^2}. \tag{1.43}$$

If, in addition, we know $(\beta_{k-1} + \alpha_{k+1})/2 \leq \gamma \leq \epsilon_k$ or $\epsilon_k \leq \gamma \leq (\beta_{k-1} + \alpha_{k+1})/2$ for some γ, then more precisely

$$\zeta_k \leq \frac{(\overline{\epsilon_k} - \gamma)(\overline{\epsilon_k} + \gamma - \beta_{k-1} - \alpha_{k+1}) + (\Delta H)_k^2}{(\gamma - \beta_{k-1})(\alpha_{k+1} - \gamma)}. \tag{1.44}$$

In particular, γ can be α'_k or β'_k. Note that all of the above holds if ϵ_k is degenerate, so long as we know the interval $(\beta_{k-1}, \alpha_{k+1})$ does not contain any eigenvalues distinct from ϵ_k.

The Kato theorem can be used by itself to obtain good lower and upper bounds to eigenvalues: One simply searches for approximate eigenvectors with small variance. But I will use the Kato theorem to supplement the Rayleigh-Ritz method: I use the Rayleigh-Ritz method to provide upper bounds to eigenvalues and approximate eigenvectors. Then the Kato theorem gives lower bounds to eigenvalues and bounds on eigenvector errors.

Note that this approach is a little odd: The Rayleigh-Ritz method minimizes $\overline{\epsilon_k}$ (within a given subspace and subject to certain orthogonality constraints), thus giving us the best available upper bound to ϵ_k. But our error estimate is derived from ΔH. Decreasing $\overline{\epsilon_k}$ might actually increase ΔH, resulting in a better upper bound but a worse lower bound.

Noting that $\Delta H \geq 0$ for any vector and $\Delta H = 0$ only for eigenvectors, one might attempt to minimize ΔH instead. But, as I have indicated in Footnote 3 above, it is computationally more efficient to diagonalize a matrix than to minimize a related function such as ΔH.

In my view, the eigenvector error is the most significant measure of an approximation and what we want to minimize. But as a practical matter, we use the Rayleigh-Ritz method to find approximate eigenvalues and eigenvectors. We minimize the approximate eigenvalue $\epsilon_k^{(n)}$ (within a given subspace and subject to

certain orthogonality constraints), a quantity which we can calculate and which we can efficiently minimize using matrix diagonalization, rather than the eigenvector error $\zeta_k^{(n)}$, a quantity which we can estimate but not calculate (unless we already know the exact eigenvector e_k), and which we cannot efficiently minimize. That the approximate eigenvalues are upper bounds is an added bonus.

A technical difficulty is that we need a rough upper bound β_{k-1} to ϵ_{k-1} and a rough lower bound α_{k+1} to ϵ_{k+1}. For β_{k-1} we can take a Rayleigh-Ritz upper bound $\overline{\epsilon_{k-1}}$ to ϵ_{k-1}. For α_{k+1} we use a variation on Temple's work due to D. H. Weinstein [Wei34]: For any vector $\overline{e}$ there is an eigenvalue ϵ satisfying

$$\langle H \rangle - \Delta H \leq \epsilon \leq \langle H \rangle + \Delta H. \tag{1.45}$$

Thus a Rayleigh-Ritz approximation $\overline{\epsilon_{k+1}}$ to e_{k+1} gives a rough lower bound $\alpha_{k+1} = \overline{\epsilon_{k+1}} - \Delta H_{k+1}$ to ϵ_{k+1}. Note that for the lowest eigenvalue ϵ_1 we take $\beta_0 = -\infty$; for the highest approximated eigenvalue ϵ_n we do not compute a lower bound.

A difficulty is that our approximations need to be sufficiently good that we can separate and identify different eigenvalues. With the choices above we know that $\epsilon_{k-1} \leq \beta_{k-1}$. We also know that $\alpha_{k+1} \leq \epsilon_{k+1}$, unless the Rayleigh-Ritz approximation to e_{k+1} is so crude that it is really an approximation to some higher eigenvector. If it happens that $\beta_{k-1} \geq \alpha_{k+1}$, then clearly our approximations are too crude. But if $\beta_{k-1} < \alpha_{k+1}$, then it may or may not be that $\beta_{k-1} < \epsilon_k < \alpha_{k+1}$. In principle, this is a difficult problem because pathological cases could arise. But, in practice, there is little difficulty and it is clear where the lowest handful of eigenvalues are roughly located. In particular, if $\Delta H_{k+1} > \frac{1}{2}(\overline{\epsilon_{k+1}} - \overline{\epsilon_k})$, that is if α_{k+1} is closer to $\overline{\epsilon_k}$ than $\overline{\epsilon_{k+1}}$, then I reject as being unreliable the lower bound α'_k to ϵ_k provided by the Kato theorem. This rule of thumb seems to work well.

In Appendix B I test my method empirically and see if bounds computed in this fashion are reliable and precise.

1.3 Optimization

We have seen that if we choose *any* complete basis for Hilbert space we can calculate approximate eigenvalues and eigenvectors. Moreover, we can estimate the

eigenvalue errors and eigenvector errors and make these arbitrarily small by choosing the subspace dimension n to be sufficiently large. But the computation requires $O(n^3)$ time: Doubling n increases the computation time by a factor of 8. On a Sun SPARCstation 1+ finding all eigenvalues and eigenvectors of a 1000×1000 matrix requires a few hours and 8 megabytes of memory using double precision arithmetic; a 2000×2000 matrix would require more than a day and 32 megabytes of memory; a 4000×4000 matrix would require more than a week and 128 megabytes of memory. In practice we are limited to $n \leq 2000$ or so. The errors in the results depend on the choice of basis vectors and can vary by many orders of magnitude for a fixed choice of n. Thus it is essential to choose the, say, 2000 basis vectors intelligently to achieve the most accurate results possible.[6]

There are two types of choices we can make to try to minimize errors for a fixed choice of n. First, given a complete basis $\{u_i\}$ we are free to reorder these basis vectors, that is to select which n we use. I have not seen any work on this issue in the quantum field theory literature. Second, the basis $\{u_i\}$ may depend on some nonlinear parameters. For example, harmonic oscillator energy eigenstates depend on the frequency ω. We can choose these parameters to try to minimize the errors. In this section I discuss in turn how to make these two types of choices so as to optimize the results.

1.3.1 Selection of Basis Vectors

Ideally, we want to select the n basis vectors that result in the "best" approximate eigenvalues and eigenvectors. But the relation between the basis vectors we select, that is the subspace $\mathcal{V}_n$, and the resulting approximate eigenvalues and eigenvectors is very complicated. Theoretically, the Weinstein function (or Weinstein determinant) describes this relation [Gou66]. But practically, the Weinstein function is of little use in developing an algorithm for selecting basis vectors. It is unfeasible to

[6] Here I assume that we use the Householder algorithm and the QL algorithm with implicit shifts or some other $O(n^3)$ method to diagonalize the matrix. There are other matrix diagonalization algorithms that require less than $O(n^3)$ time. If I were interested in producing numerical results for, say, quantum chromodynamics, then it would be advantageous to use a more efficient matrix diagonalization algorithm. Nonetheless, there would still be some practical limit to the number of basis states.

spend a lot of computational time determining the best basis vectors to select. Recall that we still have the $O(n^3)$ computation of diagonalizing an $n \times n$ matrix after we select n basis vectors. Here I take a practical approach and develop a relatively fast heuristic algorithm for selecting n reasonable basis vectors, but not necessarily the best such selection.

What do I mean by the best selection of n vectors? I could mean the selection that minimizes the approximate eigenvalue $\varepsilon_k^{(n)}$ or the selection that minimizes the eigenvalue error $\eta_k^{(n)}$. But I choose it to mean the selection that minimizes the eigenvector error $\zeta_k^{(n)}$. This concept is in a sense more fundamental and more tractable.

In particular, consider the exact eigenvector $|e_k\rangle = \sum_i |u_i\rangle\langle u_i|e_k\rangle$. With respect to the basis $\{u_i\}$ it has components $\langle u_i|e_k\rangle$. If we want to approximate e_k using only n basis vectors, then the natural and best choice is to select the n basis vectors u_i with the largest $|\langle u_i|e_k\rangle|^2$. Then the orthogonal projection of e_k onto the subspace $\mathcal{V}_n$, $P_n|e_k\rangle$, normalized to unity, is the best such approximation to e_k.

This is an attractive approach because it provides an absolute notion of the importance or value of a basis vector: The *value* of a basis vector u_i relative to the eigenvector e_k is

$$\sigma_k(i) = |\langle u_i|e_k\rangle|^2. \tag{1.46}$$

The prescription for selecting n basis vectors is to select the n with the largest values. If we increase the number of basis vectors to $n' > n$, then we select the original n basis vectors plus the $n' - n$ basis vectors with the next largest values.[7]

But the approximate eigenvector $\varepsilon_k^{(n)}$ provided by the Rayleigh-Ritz method

[7] Note that an alternative approach would be to select n basis vectors so as to minimize the approximate eigenvalue $\varepsilon_k^{(n)}$. Unfortunately, this idea could lead us to select a basis vector and later reject it. It does not provide an absolute notion of the value of a basis vector. For example, consider the hermitian operator represented by the 3×3 matrix

$$H = \begin{pmatrix} 0 & 2 & 0 \\ 2 & 3 & 12 \\ 0 & 12 & 10 \end{pmatrix}$$

with respect to the basis $\{u_1, u_2, u_3\}$. Suppose we want the minimum approximation to ε_1. If we choose just one basis vector, then u_1 ($\varepsilon_1^{(1)} = 0$) is better than u_2 ($\varepsilon_1^{(1)} = 3$) or u_3 ($\varepsilon_1^{(1)} = 10$). But if we choose two basis vectors, then u_2, u_3 ($\varepsilon_1^{(2)} = -6$) is better than u_1, u_2 ($\varepsilon_1^{(2)} = -1$) or than u_1, u_3 ($\varepsilon_1^{(2)} = 0$). For $n = 1$ we select u_1, but for $n = 2$ we reject u_1.

is, in general, not $P_n|e_k\rangle$, normalized to unity, because the Rayleigh-Ritz method, in fact, minimizes the approximate eigenvalue $\epsilon_k^{(n)}$ (within a given subspace and subject to certain orthogonality constraints), rather than the eigenvector error $\zeta_k^{(n)}$. Nevertheless, if the approximation is good, then $e_k^{(n)}$ is close to $P_n|e_k\rangle$, normalized to unity [Wei62, pp. 130–131]. And I always assume the approximation is good, because otherwise we do not care how good—or bad—our attempts at optimization are. Thus I gloss over mathematical technicalities and think of $e_k^{(n)}$ as roughly $P_n|e_k\rangle$, normalized to unity.

How do we determine the value $\sigma_k(i) = |\langle u_i|e_k\rangle|^2$? If we do not know the exact eigenvector e_k, then we cannot calculate $|\langle u_i|e_k\rangle|^2$ exactly. But if we can estimate the approximate eigenvector $\overline{e_k}$, for example, using perturbation theory, then we can use $|\langle u_i|\overline{e_k}\rangle|^2$ to estimate $|\langle u_i|e_k\rangle|^2$

In particular, my approach is to first select the basis vector with the largest, or almost largest, value. Thus we can calculate $e_1^{(1)}$. Then we use perturbation theory to estimate the values of unselected basis vectors and select the few with the largest values. Thus we can calculate $e_1^{(n)}, \ldots, e_n^{(n)}$, where $n > 1$. Then we reestimate values of still unselected basis vectors and select the few with the next largest values. Thus we can calculate $e_1^{(n')}, \ldots, e_{n'}^{(n')}$, where $n' > n$. And so on. In this way we select our basis vectors a few at a time, increasing n as we do. Since we add new basis vectors but never reject old basis vectors as we increase n, the subspace $\mathcal{V}_n$ increases monotonically. Hence the approximate eigenvalues $\epsilon_k^{(n)}$ decrease monotonically.

In general, we are interested in approximating not just one eigenvalue and eigenvector but the lowest few. It is possible to estimate each eigenvalue ϵ_k and corresponding eigenvector e_k separately, optimizing the calculation differently for each k. This is a common approach and is used, for example, by Yamazaki [Yam84]. But since the $O(n^3)$ computation of diagonalizing an $n \times n$ matrix produces n approximate eigenvalues and eigenvectors, it is advantageous to limit the number of matrix diagonalizations and approximate all desired eigenvalues and eigenvectors at once. Furthermore, we will be interested in calculating matrix elements between eigenvectors, which is difficult to do unless all eigenvectors are expressed in terms of the same basis.

Thus we begin approximating e_1. Then we increase n by adding basis vectors so as to better approximate e_1 until the eigenvector error $\zeta_1^{(n)}$ is reduced to a desired level. Then we increase n further by adding more basis vectors so as to better approximate e_2 until the eigenvector error $\zeta_2^{(n)}$ is reduced to a desired level. I assume the addition of basis vectors for e_2 does not increase the eigenvector error for e_1. If it does, then we can go back to adding more basis vectors so as to better approximate e_1. Then we improve the approximation to e_3. And so on until we have approximated all the interesting eigenvectors to the desired level of accuracy.

This is the essence of my approach to selecting basis vectors, but a few technical questions remain. First, we start the process by selecting the basis vector u_i such that $\epsilon_1^{(1)} = \langle u_i|H|u_i\rangle$ is minimum. This basis vector might not have the largest value, but this is an easy and reasonable way to begin.

Next, suppose we have already selected n basis vectors $u_1, \ldots, u_n$. We can calculate the approximate eigenvalues $\epsilon_1^{(n)}, \ldots, \epsilon_n^{(n)}$ and eigenvectors $e_1^{(n)}, \ldots, e_n^{(n)}$ by diagonalizing an $n \times n$ matrix, and estimate the eigenvector errors $\zeta_1^{(n)}, \ldots, \zeta_n^{(n)}$ using the Kato theorem. Furthermore, suppose the eigenvector errors $\zeta_1^{(n)}, \ldots, \zeta_{k-1}^{(n)}$ are all better than some desired accuracy, but $\zeta_k^{(n)} e_k^{(n+1)}$, but this is a time-consuming $O((n+1)^3)$ calculation. Instead we use perturbation theory to quickly estimate $e_k^{(n+1)}$, an eigenvector of the $(n+1) \times (n+1)$ matrix H_{n+1}. I take as an unperturbed hamiltonian

$$H_n' = P_n H P_n + |u_{n+1}\rangle\langle u_{n+1}|H|u_{n+1}\rangle\langle u_{n+1}| \tag{1.47}$$

and the perturbed hamiltonian is

$$H_{n+1} = P_{n+1} H P_{n+1} = (P_n + |u_{n+1}\rangle\langle u_{n+1}|) H (P_n + |u_{n+1}\rangle\langle u_{n+1}|). \tag{1.48}$$

The unperturbed hamiltonian is the block diagonal part of the perturbed hamiltonian (Figure 1.2).

The first-order correction to the eigenvector $e_k^{(n)}$ is

$$\Delta^{(1)} e_k^{(n)} = \frac{|u_{n+1}\rangle\langle u_{n+1}|H|e_k^{(n)}\rangle}{\epsilon_k^{(n)} - \langle u_{n+1}|H|u_{n+1}\rangle}. \tag{1.49}$$

Thus the value of u_{n+1} relative to e_k is

$$\sigma_k(n+1) = |\langle u_{n+1}|e_k\rangle|^2 \approx |\langle u_{n+1}|e_k^{(n)}\rangle|^2 \approx \left| \frac{\langle u_{n+1}|H|e_k^{(n)}\rangle}{\epsilon_k^{(n)} - \langle u_{n+1}|H|u_{n+1}\rangle} \right|^2, \tag{1.50}$$

$$
\begin{array}{c|cccc|c}
 & e_1^{(n)} & e_2^{(n)} & \cdots & e_n^{(n)} & u_{n+1} \\
\hline
e_1^{(n)} & \varepsilon_1^{(n)} & 0 & \cdots & 0 & \langle e_1^{(n)}|H|u_{n+1}\rangle \\
e_2^{(n)} & 0 & \varepsilon_2^{(n)} & \cdots & 0 & \langle e_2^{(n)}|H|u_{n+1}\rangle \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
e_n^{(n)} & 0 & 0 & \cdots & \varepsilon_n^{(n)} & \langle e_n^{(n)}|H|u_{n+1}\rangle \\
\hline
u_{n+1} & \langle u_{n+1}|H|e_1^{(n)}\rangle & \langle u_{n+1}|H|e_2^{(n)}\rangle & \cdots & \langle u_{n+1}|H|e_n^{(n)}\rangle & \langle u_{n+1}|H|u_{n+1}\rangle
\end{array}
$$

Figure 1.2: The perturbed hamiltonian H_{n+1}.

which we can calculate.[8]

Note that there is no conceptual problem with my use of perturbation theory in a variational calculation. We use perturbation theory to guide us in selecting basis vectors, but then our calculation of approximate eigenvalues and eigenvectors with the Rayleigh-Ritz method is entirely variational. We still have a method capable of giving arbitrarily accurate results.

Calculating the estimate of the value is an $O(n)$ operation, assuming we have already calculated matrix elements of the form $\langle u_i|H|u_j\rangle$. Thus estimating the value of u_{n+1} relative to e_k is a fast operation compared to the $O(n^3)$ operation of diagonalizing the matrix. Hence we can estimate the value of many different unselected basis vectors before selecting one or more of largest value, without making the time of the whole algorithm worse than $O(n^3)$.

The estimated basis vector value is nonnegative. If perturbation theory works well, then the value should be much less than one. If not, then my assumption that the approximation is already good is false. Thus the estimated values of basis vectors are probably not very good. We should add the one basis vector with largest

[8] Note that the first-order correction to the eigenvalue $\varepsilon_k^{(n)}$ is zero, but the second-order correction is

$$\Delta^{(2)}\varepsilon_k^{(n)} = \frac{|\langle u_{n+1}|H|e_k^{(n)}\rangle|^2}{\varepsilon_k^{(n)} - \langle u_{n+1}|H|u_{n+1}\rangle}.$$

If I treated eigenvalues as more fundamental than eigenvectors, then I could define the value of u_{n+1} relative to e_k to be $-\Delta^{(2)}\varepsilon_k^{(n)}$, that is the decrease in the eigenvalue. But I do not choose this approach.

estimated value, and hope that the revised approximations are significantly better.

If the estimated value is much less than one, then we can add the handful of basis vectors with largest estimated values. The squared change in $e_k^{(n)}$, and hopefully the reduction in $\zeta_k^{(n)}$, is approximately the sum of the values. If this sum is much less than one, then the perturbation calculation is probably still valid. But note that adding two or more basis vectors results in interference effects, which we neglect in our calculation of values and hope are small. In fact, the sum of the values should be less than or roughly equal to $\zeta_k^{(n)}$. Thus we have an absolute sense of what a large or small value is.

The remarks above describe my heuristic algorithm, but one technical issue remains: In principle, we can select any of an, in general, infinite number of unselected basis vectors. But, in practice, we can estimate the value of only a finite number of basis vectors. In fact, if H connects each u_i to only a finite number of u_j, then the estimated value is zero for all but a finite number of basis vectors. Nonetheless, this can be an unreasonably large number. In practice, we can estimate the value of only some basis vectors, and select the best from those we consider. In Appendix A I describe an algorithm for systematically choosing basis vectors to consider for selection.

1.3.2 Choice of Nonlinear Parameters

In general, the question of how to choose the best nonlinear parameters is a difficult one. I review the work of others and try to provide some additional insight.

Yamazaki [Yam84] uses a combination of variational and perturbative methods to calculate the energy eigenvalues of an anharmonic oscillator. He uses the harmonic oscillator basis, which depends on one nonlinear parameter, the frequency ω of the harmonic oscillator. In Chapter 2 I discuss a generalization of this basis, the weak-coupling basis. For each k he independently chooses the value of ω that minimizes $\langle u_k|H|u_k\rangle$, which he takes as an approximation to the eigenvalue ε_k. This is a reasonable approach, but leads to a different basis for each eigenvalue of interest. As I explained in the previous subsection, we want to use the same basis to approximate all eigenvalues and eigenvectors. Nonetheless, we could choose values for the nonlinear parameters that that minimize $\langle u_1|H|u_1\rangle$, where u_1 is in some physically

meaningful sense the first basis vector.

Darewych *et al.* [DHK87] also use the weak-coupling basis, both for an anharmonic oscillator and for a real scalar field theory in the infinite-volume and continuum limits. In the case of an anharmonic oscillator, they observe that the larger k is, the slower the approximate eigenvalue $\varepsilon_k^{(n)}$ converges to the exact eigenvalue ε_k as n is increased, keeping the nonlinear parameter fixed. They also observe that the larger k is, the more sensitive is $\varepsilon_k^{(n)}$ to variations in the nonlinear parameter, keeping n fixed. They recommend choosing the nonlinear parameter so as to minimize the approximate eigenvalue $\varepsilon_k^{(n)}$ for the largest value of k of interest. But they do not specify which value of n should be used when doing so.

Both Yamazaki and Darewych *et al.* focus on the eigenvalue error. But as I discussed in the previous subsection, the eigenvector error is in a sense more fundamental.

Thus consider the value $\sigma_k(i) = |\langle u_i|e_k\rangle|^2$ of the basis vector u_i relative to the eigenvector e_k. What can we say, in general, about the values $\sigma_k(i)$ for fixed k? The values are all between 0 and 1, and they sum to 1. Assume that the u_i are in order of decreasing value: $\sigma_k(1) \geq \sigma_k(2) \geq \cdots$. I hypothesize that $\sigma_k(i)$ decreases exponentially with i, keeping k fixed, at least roughly. If $\sigma_k(i)$ decreased slower, then the sum would diverge. If $\sigma_k(i)$ decreased faster, then effectively all but a finite number of $\sigma_k(i)$ would be zero, which is unlikely unless the hamiltonian is exactly solvable.

If my hypothesis is true, at least roughly, then it gives us a way to measure how good a particular basis is and to estimate how many basis vectors are needed to approximate an eigenvector to a given level of accuracy. In particular, suppose that

$$\sigma_k(i) \approx e^{-(\sigma_k i + \tau_k)}, \tag{1.51}$$

at least for large i. Then the *value* of the basis relative to the eigenvector e_k is σ_k. The larger σ_k is, the faster the basis vector values $\sigma_k(i)$ decrease as i increases, keeping k fixed. We can estimate the basis value σ_k by fitting a straight line to $\ln|\langle u_i|e_k^{(n)}\rangle|^2$, where we approximate e_k by $e_k^{(n)}$ for some moderate value of n, say, $n = 10$ or 100.

Suppose that we select the first n basis vectors. Then the approximate eigenvector is roughly $P_n|e_k\rangle$, normalized to unity, as I argued in the previous subsection.

Then the eigenvector error is

$$\zeta_k^{(n)} \approx \sum_{i=n+1}^{\infty} |\langle u_i|e_k\rangle|^2 \approx \sum_{i=n+1}^{\infty} e^{-(\sigma_k i + \tau_k)} = \frac{e^{-[\sigma_k(n+1)+\tau_k]}}{1 - e^{-\sigma_k}}. \tag{1.52}$$

If the basis value σ_k is small, then we must choose a large value of n to reduce the eigenvector error to a desired level.

So how do we choose nonlinear parameters? Suppose we are interested in only, say, the first eigenvector e_1. We fix particular values for the nonlinear parameters; calculate $e_1^{(n)}$ for some moderate value of n, using the methods of the previous subsection to select basis vectors; and estimate the basis value σ_1 using $e_1^{(n)}$. We repeat these calculations using different values for the nonlinear parameters, until we maximize the basis value σ_1. Finally, we fix the nonlinear parameters and increase n to a large value, again using the methods of the previous subsection to select basis vectors.

But we really are interested in more than one eigenvector. The observation of Darewych *et al.* regarding the convergence of approximate eigenvalues can be reexpressed using my concepts: For large i, if $k < k'$, then $\sigma_k(i) < \sigma_{k'}(i)$, that is $\sigma_k i + \tau_k > \sigma_{k'} i + \tau_{k'}$. There are two possible explanations for this phenomenon. It is possible that $\sigma_k > \sigma_{k'}$: The components of e_k decrease faster than the components of $e_{k'}$. It is also possible that $\sigma_k = \sigma_{k'}$, but $\tau_k > \tau_{k'}$: The components of e_k and $e_{k'}$ decrease at the same rate, but those of $e_{k'}$ "lag behind" those of e_k.

Empirically, the latter possibility seems more likely, as I show in Appendix B. In this case, the basis has the same value σ_k relative to any eigenvector e_k. We can define the unqualified *value* the basis as the common value of σ_k. Thus we should choose nonlinear parameters so as to maximize the value of the basis, which we can take as the value σ_1 of the basis relative to the lowest eigenvector e_1. Thus the recommendation of Darewych *et al.* for choosing the nonlinear parameters using the largest eigenvalue of interest is mistaken.

But the discussion above assumes that we are primarily interested in the asymptotic behavior of errors. In practice, we may never use an n large enough to see this behavior. For small i, the values $\sigma_k(i)$ do decrease at different rates for different k. In this case, Darewych *et al.* may be correct: We should try to minimize the value σ_k of the basis relative to the eigenvector e_k for the largest k of interest.

In this section I have described reasonable heuristic algorithms for selecting basis vectors and for choosing nonlinear parameters so as to minimize eigenvector errors. In Appendix B I test the algorithms and see if they work well in practice.

1.4 Nature of Variational Methods

In this chapter I have presented a general method for approximating eigenvalues and eigenvectors of a hermitian operator, which can, in principle, give arbitrarily accurate results. I have shown how to estimate the errors in the approximations and how to optimize the method to reduce these errors. Here I conclude by putting the method in perspective and discussing the nature of and outlook for variational methods.

In essence, all variational methods consist of somehow selecting a vector $\overline{e_k}$ in a finite-dimensional subset $\mathcal{W}$ of Hilbert space $\mathcal{V}$, which is an approximation to the exact eigenvector e_k. It is clear that the approximation will be poor unless $\mathcal{W}$ contains a good approximation to e_k. In general, $\mathcal{V}$ is infinite-dimensional: There is *a lot* of space in Hilbert space, a lot of remote corners. In order to specify e_k exactly, one has to specify an infinite number of coordinates exactly. We need to be fortunate in order to well approximate e_k with a vector in $\mathcal{W}$, that is with a finite number of coordinates.

For example, consider the 1-dimensional anharmonic oscillator discussed in Section 1.1. There we well approximated the ground state by varying only one parameter, the frequency ω. But there we knew from elementary considerations that the ground state wave function was symmetric about $q = 0$, peaked at $q = 0$ and decreased monotonically to zero as $q \to \pm\infty$. In other words, it looked more or less like a gaussian. In addition, we specified the width with ω and specified the height by requiring the wave function to be normalized to unity. Thus we pretty much knew what the wave function looked like. Perhaps our trial wave function peaked a little too low and had tails that dropped off a little too slowly, but we had roughly the correct wave function.

But consider some kind of anharmonic oscillator in, say, 1000 dimensions. The wave function depends on $\mathbf{q}$, a 1000-dimensional vector. The ground state wave function is symmetric about $\mathbf{q} = 0$, peaked at $\mathbf{q} = 0$ and decreases monotonically as $\mathbf{q} \to \infty$ in any direction. In other words, it looks more or less like a multi-dimensional gaussian:

$$\psi(\mathbf{q}) \approx \theta e^{-\frac{1}{2}\sum_i \omega_i q_i^2}, \tag{1.53}$$

where ω is a 1000-dimensional vector and θ is a normalization factor. Suppose we fine tune each of the 1000 components of ω to get the width of the gaussian about right in each dimension. As in the 1-dimensional case, our trial wave function does not peak quite right or drop off quite right. So there is a small error *in each dimension.* But 1000 small errors add up to a big error! Even though we have fine tuned 1000 parameters, our approximation is not very good at all.

The problem is that infinite-dimensional Hilbert spaces have a lot of space—and some have a lot more than others. The Hilbert space for the 1-dimensional oscillator is infinite-dimensional, but in some loose sense it is effectively low-dimensional: The ground state for any reasonable potential can be well approximated by specifying only, say, 10 parameters. But the Hilbert space for the the 1000-dimensional oscillator is "1000 times more infinite" than the Hilbert space for the 1-dimensional oscillator.[9] It is effectively high-dimensional in the sense that we probably need to specify more than $1000 \times 10 = 10000$ parameters to well approximate the ground state.

There are a couple of points here. First, we cannot use variational methods blindly and expect good results. We need to use all available physical insight to come up with a subset $\mathcal{W}$ of trial vectors that have a reasonable chance of being close to the desired eigenvectors. Second, variational methods will not work very well if the Hilbert space is effectively very large, unless by chance a desired eigenvector is near one of our trial vectors, for example, near a gaussian.

For example, the Hilbert space for a real scalar quantum field theory in $1+1$ spacetime dimensions in the continuum limit with finite volume is "infinitely more infinite" than the Hilbert space for the 1-dimensional oscillator. And with infinite volume it is "infinitely, infinitely more infinite." It is naïve to suppose we could do much by varying just a handful of parameters: Hilbert space is just too big. A

[9] The Hilbert space $\mathcal{V}^{1000}$ for the 1000-dimensional oscillator is the 1000-fold tensor product of the Hilbert space $\mathcal{V}^1$ for the 1-dimensional oscillator: $\mathcal{V}^{1000} = \mathcal{V}^1 \otimes \cdots \otimes \mathcal{V}^1$. If the *dimension* of $\mathcal{V}^1$ is n, then the *dimension* of $\mathcal{V}^{1000}$ is n^{1000}.

reflection of this problem is the insignificance of finite energy excitations compared to the infinite ground state energy noted by Darewych *et al.* [DHK87]. Another reflection is Feynman's frustration with the sensitivity to high frequencies: He tried to adjust the physically interesting low frequencies in trial wave functions, but his results were swamped out by high frequency effects [Fey87].

I am convinced that all attempts to apply variational methods directly to quantum field theory in the continuum limit are hopeless. But variational methods applied to finite models of quantum field theory, for example, quantum field theory on a finite lattice, have some hope of success. It all depends on how effectively large the Hilbert space is. If the theory can be well modeled by a lattice theory with, say, 10 points, then variational methods can be successful. But if, say, 10000 points are required, then variational methods are hopeless. The problem is that for most classes of quantum field theories, we can choose values for coupling constants such that there are interesting phenomena at many different length scales. In this case, we need many lattice points to well model the physics and variational methods fail.[10]

In particular, it might be that quantum chromodynamics is an extremely complicated theory that cannot be modeled by just a handful of parameters. Variational methods—and perhaps all other methods—might simply not work. The world might be a stranger place than we can describe.

But I am getting ahead of myself. Variational methods certainly work for free field theories, in which all of the eigenstates are gaussian wave functions. And I expect variational methods to work for a class of quantum field theories with coupling constants in certain ranges. In the following chapters I attempt to realize that expectation.

[10] But see Wilson's ideas about lattices in [Wil89].

Chapter 2

Hamiltonian Lattice Field Theory

In Chapter 1 I developed a general method for finding approximate eigenvalues and eigenvectors of a hermitian operator. The method requires a hermitian operator H on a Hilbert space $\mathcal{V}$, a complete orthonormal basis $\{u_i\}$ for $\mathcal{V}$, and matrix elements $\langle u_i|H|u_j\rangle$. If we want to estimate errors, we also need the variance $(\Delta H)^2$ of each approximate eigenvector. In this chapter I discuss a class of theories, real scalar quantum field theories on a finite lattice, to which I apply the method. In Section 2.1 I introduce the hamiltonian formulation of the theories. In Section 2.2 I discuss various bases I might use and argue for a particular choice, the weak-coupling basis. In Section 2.3 I describe how to calculate matrix elements, variances and other interesting quantities using the weak-coupling basis.

2.1 Real Scalar Quantum Field Theory

Since my aim is not to solve a particular theory, such as quantum chromodynamics, but to develop a general method for solving any theory, I apply my method to the simplest class of quantum field theories: theories of a single real scalar field. This class includes theories with interesting phenomena, such as bound states and spontaneous symmetry breaking. The generalization to several bosonic or fermionic fields is straightforward, but I prefer to avoid the technical complications of several fields. This section reviews real scalar quantum field theory, first as an infinite-volume,

continuum theory and then as a finite-volume, lattice theory. The key results are Equations (2.25), (2.26c), (2.27) and (2.28c), which describe the finite-volume, lattice theory in terms of free particle destruction and creation operators.

2.1.1 Infinite-Volume, Continuum Theory

I begin by presenting the theory in the infinite-volume and continuum limits. I work in a spacetime with d dimensions: $d-1$ spatial dimensions, which are unbounded and continuous, and 1 temporal dimension, which is unbounded and continuous. The metric on spacetime is $g_{\mu\nu}$. I assume spacetime is flat:

$$g_{\mu\nu} = \mathrm{diag}\{+1, \underbrace{-1, \ldots, -1}_{d-1 \text{ times}}\}. \tag{2.1}$$

Note that I work in units such that $\hbar = c = 1$.

The real scalar field ϕ is defined at each spacetime point x, and is unbounded and continuous.

The theory is defined by the lagrangian density

$$\mathcal{L} = \tfrac{1}{2}\lambda_\phi \partial_\mu\phi\partial^\mu\phi - V(\phi), \tag{2.2}$$

where λ_ϕ is a coupling constant and $V(\phi)$ is a potential density. I assume V is an entire function of ϕ, that is V has a power series expansion in ϕ with an infinite radius of convergence:

$$V(\phi) = \sum_{k=0}^{\infty} \lambda_k \lambda_\phi^{k/2} \phi^k. \tag{2.3}$$

I have introduced factors of λ_ϕ for later convenience: Changing λ_ϕ is equivalent to rescaling the field ϕ. The theory is a free theory for a particle with mass m if $V(\phi) = \frac{1}{2}m^2\lambda_\phi\phi^2$. In the special case of $d = 0+1$ spacetime dimensions, the theory describes a single particle of mass λ_ϕ in the potential $V(\phi)$, where ϕ is the 1-dimensional position of the particle.

The energy-momentum tensor is

$$\Theta^{\mu\nu} = \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\partial^\nu\phi - g^{\mu\nu}\mathcal{L} = \lambda_\phi\partial^\mu\phi\partial^\nu\phi - g^{\mu\nu}\mathcal{L}. \tag{2.4}$$

Since the lagrangian density does not depend explicitly on the spacetime point x, the energy-momentum tensor is a set of conserved currents. In particular, the total energy at time t,

$$H = \int d^{d-1}\mathbf{x}\,\Theta^{00} = \int d^{d-1}\mathbf{x}\left[\tfrac{1}{2}\lambda_\phi\dot{\phi}^2 + \tfrac{1}{2}\lambda_\phi(\nabla\phi)^2 + \sum_{k=0}^{\infty}\lambda_k\lambda_\phi^{k/2}\phi^k\right], \tag{2.5}$$

and the ith component of the total momentum at time t,

$$P_i = \int d^{d-1}\mathbf{x}\,\Theta^{0i} = -\int d^{d-1}\mathbf{x}\,\lambda_\phi\dot{\phi}\partial_i\phi, \tag{2.6}$$

are conserved quantities. As usual, $\dot{\phi} = \partial_0\phi$ is the time-derivative of ϕ.

The canonical momentum density conjugate to ϕ is

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\phi}} = \lambda_\phi\dot{\phi}. \tag{2.7}$$

The hamiltonian describes a quantum theory if we interpret ϕ and π as operators on a Hilbert space that satisfy the canonical commutation relations at time t,

$$[\phi(\mathbf{x}), \pi(\mathbf{x}')] = i\delta^{d-1}(\mathbf{x}-\mathbf{x}'), \qquad [\phi(\mathbf{x}), \phi(\mathbf{x}')] = [\pi(\mathbf{x}), \pi(\mathbf{x}')] = 0. \tag{2.8}$$

The hamiltonian of the theory at time t is the total energy expressed as a function of ϕ and π:

$$H = \int d^{d-1}\mathbf{x}\left[\tfrac{1}{2}\lambda_\phi^{-1}\pi^2 + \tfrac{1}{2}\lambda_\phi(\nabla\phi)^2 + \sum_{k=0}^{\infty}\lambda_k\lambda_\phi^{k/2}\phi^k\right]. \tag{2.9}$$

Similarly, the ith component of the total momentum at time t expressed as a function of ϕ and π is

$$P_i = -\int d^{d-1}\mathbf{x}\,\frac{\pi(\partial_i\phi) + (\partial_i\phi)\pi}{2}. \tag{2.10}$$

The momentum $\mathbf{p}$ is a vector in an unbounded and continuous $(d-1)$-dimensional space, the dual space of physical space. I define the spatial Fourier transforms $\tilde{\phi}$ and $\tilde{\pi}$ of ϕ and π, respectively, at time t:

$$\tilde{\phi}(\mathbf{p}) = \int d^{d-1}\mathbf{x}\,\phi(\mathbf{x})e^{-i\mathbf{p}\cdot\mathbf{x}}, \qquad \phi(\mathbf{x}) = \int \frac{d^{d-1}\mathbf{p}}{(2\pi)^{d-1}}\,\tilde{\phi}(\mathbf{p})e^{+i\mathbf{p}\cdot\mathbf{x}}, \tag{2.11a}$$

$$\tilde{\pi}(\mathbf{p}) = \int d^{d-1}\mathbf{x}\,\pi(\mathbf{x})e^{-i\mathbf{p}\cdot\mathbf{x}}, \qquad \pi(\mathbf{x}) = \int \frac{d^{d-1}\mathbf{p}}{(2\pi)^{d-1}}\,\tilde{\pi}(\mathbf{p})e^{+i\mathbf{p}\cdot\mathbf{x}}. \tag{2.11b}$$

They satisfy the commutation relations at time t,

$$[\tilde{\phi}(\mathbf{p}), \tilde{\pi}(\mathbf{p}')] = i(2\pi)^{d-1}\delta^{d-1}(\mathbf{p}+\mathbf{p}'), \qquad [\tilde{\phi}(\mathbf{p}), \tilde{\phi}(\mathbf{p}')] = [\tilde{\pi}(\mathbf{p}), \tilde{\pi}(\mathbf{p}')] = 0. \tag{2.12}$$

Since ϕ and π are real (hermitian), $\tilde{\phi}^\dagger(\mathbf{p}) = \tilde{\phi}(-\mathbf{p})$ and $\tilde{\pi}^\dagger(\mathbf{p}) = \tilde{\pi}(-\mathbf{p})$.

In terms of $\tilde{\phi}$ and $\tilde{\pi}$, the hamiltonian at time t is

$$H = \int \frac{d^{d-1}\mathbf{p}}{(2\pi)^{d-1}} \left(\tfrac{1}{2}\lambda_\phi^{-1}\tilde{\pi}^\dagger\tilde{\pi} + \tfrac{1}{2}|\mathbf{p}|^2\lambda_\phi\tilde{\phi}^\dagger\tilde{\phi}\right)$$
$$+ \sum_{k=0}^{\infty} \lambda_k \lambda_\phi^{k/2} \int \frac{d^{d-1}\mathbf{p}_1}{(2\pi)^{d-1}} \cdots \frac{d^{d-1}\mathbf{p}_k}{(2\pi)^{d-1}} (2\pi)^{d-1}\delta^{d-1}(\mathbf{p}_1 + \cdots + \mathbf{p}_k)\, \tilde{\phi}(\mathbf{p}_1)\cdots\tilde{\phi}(\mathbf{p}_k) \quad (2.13)$$

and the ith component of the total momentum at time t is

$$P_i = -i \int \frac{d^{d-1}\mathbf{p}}{(2\pi)^{d-1}}\, p_i \frac{\tilde{\pi}^\dagger\tilde{\phi} - \tilde{\phi}^\dagger\tilde{\pi}}{2}. \quad (2.14)$$

In order to define free particle destruction and creation operators, I introduce an *arbitrary* parameter μ, the mass of fictitious free particles, and divide H into a free part $H_{\text{free}}(\mu)$ and an interacting part $H_{\text{int}}(\mu)$:

$$H = H_{\text{free}}(\mu) + H_{\text{int}}(\mu), \quad (2.15)$$
$$H_{\text{free}}(\mu) = \int d^{d-1}\mathbf{x} \left[\tfrac{1}{2}\lambda_\phi^{-1}\pi^2 + \tfrac{1}{2}\lambda_\phi(\nabla\phi)^2 + \tfrac{1}{2}\mu^2\lambda_\phi\phi^2\right], \quad (2.16)$$
$$H_{\text{int}}(\mu) = \int d^{d-1}\mathbf{x} \left[-\tfrac{1}{2}\mu^2\lambda_\phi\phi^2 + \sum_{k=0}^{\infty}\lambda_k\lambda_\phi^{k/2}\phi^k\right]. \quad (2.17)$$

Then I define the destruction operator $a(\mathbf{p})$ and the creation operator $a^\dagger(\mathbf{p})$ for a free particle with momentum $\mathbf{p}$ at time t in the theory described by $H_{\text{free}}(\mu)$:

$$a(\mathbf{p}) = \frac{1}{\sqrt{2}} L^{-(d-1)/2} \left[\sqrt{\omega(\mathbf{p})\lambda_\phi}\,\tilde{\phi}(\mathbf{p}) + \frac{i}{\sqrt{\omega(\mathbf{p})\lambda_\phi}}\tilde{\pi}(\mathbf{p})\right], \quad (2.18a)$$
$$a^\dagger(\mathbf{p}) = \frac{1}{\sqrt{2}} L^{-(d-1)/2} \left[\sqrt{\omega(\mathbf{p})\lambda_\phi}\,\tilde{\phi}(-\mathbf{p}) - \frac{i}{\sqrt{\omega(\mathbf{p})\lambda_\phi}}\tilde{\pi}(-\mathbf{p})\right], \quad (2.18b)$$
$$\tilde{\phi}(\mathbf{p}) = \frac{1}{\sqrt{2\omega(\mathbf{p})\lambda_\phi}} L^{(d-1)/2}[a(\mathbf{p}) + a^\dagger(-\mathbf{p})], \quad (2.18c)$$
$$\tilde{\pi}(\mathbf{p}) = -i\sqrt{\frac{\omega(\mathbf{p})\lambda_\phi}{2}}\, L^{(d-1)/2}[a(\mathbf{p}) - a^\dagger(-\mathbf{p})], \quad (2.18d)$$

where

$$\omega(\mathbf{p}) = \sqrt{|\mathbf{p}|^2 + \mu^2} \quad (2.19)$$

is the energy of a free particle with momentum $\mathbf{p}$. The destruction and creation operators satisfy the commutation relations at time t,

$$[a(\mathbf{p}), a^\dagger(\mathbf{p}')] = L^{-(d-1)}(2\pi)^{d-1}\delta^{d-1}(\mathbf{p}-\mathbf{p}'), \quad [a(\mathbf{p}), a(\mathbf{p}')] = [a^\dagger(\mathbf{p}), a^\dagger(\mathbf{p}')] = 0. \quad (2.20)$$

Here L^{d-1} is the volume of space, which for now I take to be infinite. Thus a and $a^\dagger$ are, strictly speaking, not well defined. But as defined they are dimensionless. In the next subsection we see that this definition leads to convenient commutation relations in the finite-volume theory, Equation (2.25).

In terms of a and $a^\dagger$, the hamiltonian at time t is

$$H = L^{d-1} \int \frac{d^{d-1}\mathbf{p}}{(2\pi)^{d-1}}\, \omega(\mathbf{p})\left[a^\dagger(\mathbf{p})a(\mathbf{p}) + \tfrac{1}{2}\right]$$
$$+ \sum_{k=0}^{\infty} 2^{-k/2}\left(\lambda_k - \tfrac{1}{2}\mu^2\delta_{k,2}\right) L^{(k/2)(d-1)} \int \frac{d^{d-1}\mathbf{p}_1}{(2\pi)^{d-1}} \cdots \frac{d^{d-1}\mathbf{p}_k}{(2\pi)^{d-1}}$$
$$\times \Big\{(2\pi)^{d-1}\delta^{d-1}(\mathbf{p}_1 + \cdots + \mathbf{p}_k)\,\omega(\mathbf{p}_1)^{-1/2}\cdots\omega(\mathbf{p}_k)^{-1/2}$$
$$\times [a(\mathbf{p}_1) + a^\dagger(-\mathbf{p}_1)]\cdots[a(\mathbf{p}_k) + a^\dagger(-\mathbf{p}_k)]\Big\}, \quad (2.21)$$

where the $-\frac{1}{2}\mu^2\lambda_\phi\phi^2$ term in $H_{\text{int}}(\mu)$ is absorbed into the λ_2 term. Similarly, the ith component of the total momentum at time t is

$$P_i = L^{d-1} \int \frac{d^{d-1}\mathbf{p}}{(2\pi)^{d-1}}\, p_i\, a^\dagger(\mathbf{p})a(\mathbf{p}). \quad (2.22)$$

Observe that all factors of λ_ϕ have disappeared in H and P_i.

Finally, note that each component P_i of the total momentum is conserved. In addition, if the potential density $V(\phi)$ is even in ϕ, $V(-\phi) = V(\phi)$, that is if $V(\phi)$ involves only even powers of ϕ, then parity is also conserved. Thus Hilbert space breaks into sectors of definite momentum and, if V is even in ϕ, definite parity. The hamiltonian can be viewed as a block diagonal matrix, one block per sector. When I apply the methods of Chapter 1, I will always focus attention on a specific sector and treat H as being restricted to that sector. For example, I will look for energy eigenstates with zero total momentum and even parity. In Section 2.2 I look for a basis for Hilbert space that reflects the symmetries of the system.

2.1.2 Finite-Volume, Lattice Theory

I argued in Section 1.4 that variational methods applied to quantum field theory have no hope of success unless applied to finite models of the theory. Furthermore, the infinite-volume and/or continuum forms of the theory are plagued with various divergences and renormalization problems, which make them unsuitable for

Infinite Volume		Finite Volume
$\int \frac{d^{d-1}\mathbf{p}}{(2\pi)^{d-1}}$	$\longleftrightarrow$	$L^{-(d-1)}\sum_{\mathbf{p}}$
$(2\pi)^{d-1}\delta^{d-1}(\mathbf{p})$	$\longleftrightarrow$	$L^{d-1}\delta_{\mathbf{p}}$
$(2\pi)^{d-1}\frac{\delta}{\delta\tilde{\phi}(\mathbf{p})}$	$\longleftrightarrow$	$L^{d-1}\frac{\partial}{\partial\tilde{\phi}_{\mathbf{p}}}$

Table 2.1: Translations between the infinite-volume and finite-volume theories.

numerical methods. Here I rewrite the real scalar quantum field theory discussed above as one on a finite lattice. We do not need to rederive the theory: We merely need to reinterpret the formulae for the infinite-volume, continuum theory as formulae for the finite-volume, lattice theory.

Suppose space rather than being unbounded is bounded with extent L in each dimension. Thus the volume of space is L^{d-1}. We approach the infinite-volume limit as $L \to \infty$. I impose periodic boundary conditions on space by identifying each point $\mathbf{x}$ with the point $\mathbf{x} + L\hat{\imath}$, where $\hat{\imath}$ is a unit vector in the ith direction. All formulae involving $\mathbf{x}$ are unchanged, except that spatial integrals are now over a finite volume, and we need to keep in mind the periodic boundary conditions when interpreting spatial delta functions and derivatives.

If physical space is bounded, then momentum space, the dual space, is discrete with lattice spacing $2\pi/L$. In particular, each component p_i is $2\pi/L$ times an integer. We need to reinterpret momentum integrals as sums, momentum Dirac delta functions as Kronecker deltas, and functional derivatives with respect to functions of $\mathbf{p}$ as partial derivatives. The translations between the infinite-volume and finite-volume theories are summarized in Table 2.1.

Suppose space rather than being continuous is a discrete lattice with spacing a. Thus the volume of a lattice cell is a^{d-1}. In particular, suppose each component x_i is a times an integer. Then we need to reinterpret spatial integrals as sums, spatial Dirac delta functions as Kronecker deltas, functional derivatives with respect to functions of $\mathbf{x}$ as partial derivatives, and spatial derivatives as finite differences. The translations between the continuum and lattice theories are summarized in Table 2.2.

Continuum		Lattice
$\int d^{d-1}\mathbf{x}$	$\longleftrightarrow$	$a^{d-1}\sum_{\mathbf{x}}$
$\delta^{d-1}(\mathbf{x})$	$\longleftrightarrow$	$a^{-(d-1)}\delta_{\mathbf{x}}$
$\frac{\delta}{\delta\phi(\mathbf{x})}$	$\longleftrightarrow$	$a^{-(d-1)}\frac{\partial}{\partial\phi_{\mathbf{x}}}$
$\partial_i\phi(\mathbf{x})$	$\longleftrightarrow$	$a^{-1}(\phi_{\mathbf{x}+a\hat{\imath}} - \phi_{\mathbf{x}})$
$\lvert\mathbf{p}\rvert^2$	$\longleftrightarrow$	$a^{-2}\sum_i [2 - 2\cos(p_i a)]$

Table 2.2: Translations between the continuum and lattice theories.

If physical space is discrete, then momentum space, the dual space of physical space, is bounded with extent $2\pi/a$ in each dimension. We approach the continuum limit, that is the infinite momentum cutoff limit, as $a \to 0$. Then momentum space has periodic boundary conditions: Each point $\mathbf{p}$ is identified with the point $\mathbf{p} + (2\pi/a)\hat{\imath}$. All formulae involving $\mathbf{p}$ are unchanged, except that momentum integrals are now over finite volume, and we need to keep in mind the periodic boundary conditions when interpreting momentum delta functions.

Note that the correspondences between the infinite-volume and finite-volume theories or the continuum and lattice theories are such that all quantities retain the same engineering dimensions.

We could consider a finite-volume, continuum theory ($L < \infty, a = 0$) or an infinite-volume, lattice theory ($L = \infty, a > 0$), but I want to consider finite-volume, lattice theories ($L < \infty, a > 0$). In this case, L and a are related: L/a is an integer, the number of lattice points in any given direction. The total number of lattice points is $N = (L/a)^{d-1}$. The total number of momenta is also $N = [(2\pi/a)/(2\pi/L)]^{d-1}$.

As an example of the translation of formulae from the infinite-volume, continuum theory to the finite-volume, lattice theory, the commutation relations (2.8), (2.12) and (2.20) at time t translate to:

$$[\phi_{\mathbf{x}}, \pi_{\mathbf{x}'}] = ia^{-(d-1)}\delta_{\mathbf{x},\mathbf{x}'}, \qquad [\phi_{\mathbf{x}}, \phi_{\mathbf{x}'}] = [\pi_{\mathbf{x}}, \pi_{\mathbf{x}'}] = 0, \tag{2.23}$$

$$[\tilde{\phi}_{\mathbf{p}}, \tilde{\pi}_{\mathbf{p}'}] = iL^{d-1}\delta_{\mathbf{p},-\mathbf{p}'}, \qquad [\tilde{\phi}_{\mathbf{p}}, \tilde{\phi}_{\mathbf{p}'}] = [\tilde{\pi}_{\mathbf{p}}, \tilde{\pi}_{\mathbf{p}'}] = 0, \tag{2.24}$$

$$[a_{\mathbf{p}}, a^\dagger_{\mathbf{p}'}] = \delta_{\mathbf{p},\mathbf{p}'}, \qquad [a_{\mathbf{p}}, a_{\mathbf{p}'}] = [a^\dagger_{\mathbf{p}}, a^\dagger_{\mathbf{p}'}] = 0. \tag{2.25}$$

Similarly, Equations (2.9), (2.13) and (2.21) for the hamiltonian at time t translate to:

$$H = a^{d-1} \sum_{\mathbf{x}} \left[\tfrac{1}{2}\lambda_\phi^{-1}\pi_{\mathbf{x}}^2 + \tfrac{1}{2}a^{-2}\lambda_\phi \sum_i (\phi_{\mathbf{x}+a\hat{i}} - \phi_{\mathbf{x}})^2 + \sum_{k=0}^{\infty} \lambda_k \lambda_\phi^{k/2} \phi_{\mathbf{x}}^k \right] \tag{2.26a}$$

$$= L^{-(d-1)} \sum_{\mathbf{p}} \left\{ \tfrac{1}{2}\lambda_\phi^{-1} \tilde{\pi}^\dagger_{\mathbf{p}} \tilde{\pi}_{\mathbf{p}} + \tfrac{1}{2}a^{-2}\lambda_\phi \sum_i [2 - 2\cos(p_i a)]\, \tilde{\phi}^\dagger_{\mathbf{p}} \tilde{\phi}_{\mathbf{p}} \right\}$$
$$+ \sum_{k=0}^{\infty} \lambda_k \lambda_\phi^{k/2} L^{(1-k)(d-1)} \sum_{\mathbf{p}_1,\ldots,\mathbf{p}_k} \delta_{\mathbf{p}_1+\cdots+\mathbf{p}_k}\, \tilde{\phi}_{\mathbf{p}_1} \cdots \tilde{\phi}_{\mathbf{p}_k} \tag{2.26b}$$

$$= \sum_{\mathbf{p}} \omega_{\mathbf{p}} \left(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + \tfrac{1}{2} \right)$$
$$+ \sum_{k=0}^{\infty} 2^{-k/2} \left(\lambda_k - \tfrac{1}{2}\mu^2 \delta_{k,2} \right) L^{(1-k/2)(d-1)}$$
$$\times \sum_{\mathbf{p}_1,\ldots,\mathbf{p}_k} \delta_{\mathbf{p}_1+\cdots+\mathbf{p}_k}\, \omega_{\mathbf{p}_1}^{-1/2} \cdots \omega_{\mathbf{p}_k}^{-1/2} (a_{\mathbf{p}_1} + a^\dagger_{-\mathbf{p}_1}) \cdots (a_{\mathbf{p}_k} + a^\dagger_{-\mathbf{p}_k}), \tag{2.26c}$$

where Equation (2.19) for the energy of a free particle with momentum $\mathbf{p}$ translates to:

$$\omega_{\mathbf{p}} = \sqrt{a^{-2} \sum_i [2 - 2\cos(p_i a)] + \mu^2}. \tag{2.27}$$

Finally, Equations (2.10), (2.14) and (2.22) for the ith component of the total momentum at time t translate to:[1]

$$P_i = -a^{d-2} \sum_{\mathbf{x}} \frac{\pi_{\mathbf{x}}(\phi_{\mathbf{x}+a\hat{i}} - \phi_{\mathbf{x}}) + (\phi_{\mathbf{x}+a\hat{i}} - \phi_{\mathbf{x}})\pi_{\mathbf{x}}}{2} \tag{2.28a}$$

$$= -iL^{(d-1)} \sum_{\mathbf{p}} p_i \frac{\tilde{\pi}^\dagger_{\mathbf{p}} \tilde{\phi}_{\mathbf{p}} - \tilde{\phi}^\dagger_{\mathbf{p}} \tilde{\pi}_{\mathbf{p}}}{2} \tag{2.28b}$$

$$= \sum_{\mathbf{p}} p_i\, a^\dagger_{\mathbf{p}} a_{\mathbf{p}}. \tag{2.28c}$$

[1] In fact, since space is now discrete, Noether's theorem fails for P_i: P_i in terms of ϕ and π, Equation (2.28a), is *not* conserved, as can be directly verified. Nevertheless, P_i in terms of $\tilde{\phi}$ and $\tilde{\pi}$, Equation (2.28b), and P_i in terms of a and $a^\dagger$, Equation (2.28c), are equal and are conserved, as is clear from the latter expression. The discrepancy is explained by observing that whereas P_i in terms of ϕ and π is an exact translation of the corresponding expression in the infinite-volume, continuum theory, P_i in terms of $\tilde{\phi}$ and $\tilde{\pi}$ or a and $a^\dagger$ is not. In the exact translation, p_i would be replaced by $a^{-1}\sin(p_i a)$. Thus I will use P_i only in terms of $\tilde{\phi}$ and $\tilde{\pi}$ or a and $a^\dagger$, since these forms are conserved, and not worry about their origin. Note that there is no similar problem with the hamiltonian, since time is still continuous.

In this section I introduced real scalar quantum field theory on a finite lattice, which is specified by the hamiltonian (2.26). The theory describes N identical oscillators, one at each lattice point, with nearest neighbors being coupled together. Two viewpoints are possible. The first is that the theory is a well defined, finite quantum mechanical theory of coupled oscillators. The theory is unrelated to any quantum field theory but is interesting in its own right. In this case there is no difficulty in interpretation: We are interested in finding energy eigenvalues and eigenstates, which corresponds to different modes of the oscillators. I take this viewpoint in Appendix B, where I present numerical results of applying the method to simple quantum mechanical systems.

The second viewpoint is that the theory is a finite approximation to some infinite-volume, continuum theory. In this case we want to interpret the theory in terms of physical particles, bound states and scattering amplitudes, which I show how to do in Chapter 3.

2.2 Choice of Basis

Now that we have a hamiltonian H on a Hilbert space $\mathcal{V}$, we need to choose a complete, preferably orthonormal basis $\{u_i\}$ for $\mathcal{V}$. In this section I consider a few different bases that could be used, and argue for my choice, the weak-coupling basis.

There are a few criteria that guide the choice: First, of course, the basis must be complete—a finite number of *ad hoc* parameters that describe a finite-dimensional submanifold of $\mathcal{V}$ do not lead to a systematic calculation, one that can achieve arbitrary accuracy. Second, the basis must permit numerical calculation: A computer can only store and manipulate a finite number of quantities. Third, the basis should reflect the symmetries of the system, that is each basis state should have definite momentum and parity. Lastly, the basis should be "good" in the sense of Section 1.4, that is it should be possible to well approximate the lowest several eigenstates of the system using a small number of basis states. To this end it is helpful if the basis depends on one or more nonlinear parameters that can be adjusted to better fit the basis to the system.

In general, a basis for Hilbert space is determined by a complete set $\{O_i\}$ of

commuting operators. Then the basis consists of states $|\{o_i\}\rangle$ that are simultaneous eigenstates: $O_k|\{o_i\}\rangle = o_k|\{o_i\}\rangle$ for each k. A basis state is fixed by specifying an eigenvalue o_i of the operator O_i for each i.

2.2.1 Configuration and Conjugate Momentum Bases

For example, the operators $\{\phi_{\mathbf{x}}\}$, or equivalently $\{\tilde{\phi}_{\mathbf{p}}\}$, determine a basis, the *configuration basis*. In particular, a basis state $|\phi\rangle$ is fixed by specifying the field value $\phi_{\mathbf{x}}$ for each point $\mathbf{x}$. Recall that $\mathbf{x}$ can be any one of N lattice points. Then an arbitrary state is

$$|\psi\rangle = \int d^N\phi\, |\phi\rangle\langle\phi|\psi\rangle, \tag{2.29}$$

where $\psi(\phi) = \langle\phi|\psi\rangle$ is the configuration wave function.

Unfortunately, the configuration basis is unsuitable for numerical methods: Each basis state $|\phi\rangle$ is unnormalizable and corresponds to a Dirac delta wave function. The problem is that the spectrum of each operator $\phi_{\mathbf{x}}$ is continuous. Only superpositions of an infinite number of basis states, that is wave functions that are nonzero for an infinite number of configurations, are normalizable. But a computer cannot directly store or manipulate such a function.

Similarly, the operators $\{\pi_{\mathbf{x}}\}$, or equivalently $\{\tilde{\pi}_{\mathbf{p}}\}$, determine a basis, the *conjugate momentum basis*. But this basis is also not suitable for numerical methods.

2.2.2 Hamiltonian Power Basis

Another possible basis is the set $\{H^k|\psi_0\rangle : k = 0, 1, \ldots\}$, the *hamiltonian power basis*, where ψ_0 is some state that has nonzero overlap with the lowest energy eigenstate e_1 within a particular sector: $\langle e_1|\psi_0\rangle \neq 0$. This basis is suggested by considering the heat kernel $e^{-tH} = \sum_k \frac{1}{k!}(-t)^k H^k$, which projects out the lowest energy eigenstate within a given sector in the limit $t \to \infty$. Duncan and Roskies purport to use this basis [DR85a, DR85b, Dun85, Dun87], but, in fact, use a different but related basis. A problem is that $H^k|\psi_0\rangle$ is very difficult to calculate for even modest k. More importantly, the hamiltonian power basis is, in general, not complete. It can be used to approximate the lowest energy state within a particular sector to

arbitrary accuracy, but not necessarily excited states. Thus this basis cannot be used for a systematic calculation of approximations to excited states.

2.2.3 Strong-Coupling Basis

A promising basis is the *strong-coupling basis*. We can rewrite the hamiltonian (2.26a) as

$$H = \sum_{\mathbf{x}} H_{\mathbf{x}} + H_{\text{con}}, \tag{2.30}$$

$$H_{\mathbf{x}} = a^{d-1}\left[\tfrac{1}{2}\lambda_\phi^{-1}\pi_{\mathbf{x}}^2 + (d-1)a^{-2}\lambda_\phi\phi_{\mathbf{x}}^2 + \sum_{k=0}^{\infty}\lambda_k\lambda_\phi^{k/2}\phi_{\mathbf{x}}^k\right], \tag{2.31}$$

$$H_{\text{con}} = -a^{d-3}\lambda_\phi \sum_{\mathbf{x}}\sum_i \phi_{\mathbf{x}}\phi_{\mathbf{x}+a\hat{i}}. \tag{2.32}$$

The Hilbert space $\mathcal{V}$ is the tensor product of identical Hilbert spaces, one for each lattice point: $\mathcal{V} = \bigotimes_{\mathbf{x}} \mathcal{V}_{\mathbf{x}}$. Each hamiltonian $H_{\mathbf{x}}$ acts on the corresponding Hilbert space $\mathcal{V}_{\mathbf{x}}$. Thus H can be separated into a sum of identical one-dimensional quantum mechanical hamiltonians $H_{\mathbf{x}}$, one for each lattice point, except a piece H_{con} that connects adjacent lattice points is left over. The strong-coupling basis is determined by the commuting operators $\{H_{\mathbf{x}}\}$. In particular, if $\{e_k\}$ is a set of eigenstates for $H_{\mathbf{x}}$, then a basis state $|k\rangle$ is fixed by specifying $k_{\mathbf{x}}$ for each lattice point $\mathbf{x}$, that is by choosing an eigenstate $e_{k_{\mathbf{x}}}$ of $H_{\mathbf{x}}$ at each lattice point $\mathbf{x}$.

The strong-coupling basis is amenable to numerical methods. Moreover, the basis is "good" to the extent that the eigenstates e_k of $H_{\mathbf{x}}$ reflect the coupling constants of the system. Also, we expect the basis to work well when H_{con} is negligible, that is in the strong-coupling limit.

But the basis has a few problems. First, we must compute eigenvalues and eigenstates of $H_{\mathbf{x}}$, a one-dimensional quantum mechanical hamiltonian, and compute the $\phi_{\mathbf{x}}\phi_{\mathbf{x}+a\hat{i}}$ matrix elements between these eigenstates. In general, this can be done numerically to high accuracy, for example, by solving the ordinary differential equation associated with $H_{\mathbf{x}}$ and then evaluating integrals to get matrix elements. This is not a real problem, but merely a messy technical issue.

Second, the basis states have definite parity but not definite momentum. Nevertheless, states of definite momentum can be constructed by superposing spatial

translations of a single state. Again, this is not a real problem, but merely a technical complication.

Third, the basis states reflect primarily short-range correlations, that is high-momentum behavior. If a basis state has excitations at only a few lattice points, then it will have correlations over distances of only a few lattice spacings. Since we are mainly interested in long-range, that is low-momentum, behavior, the strong-coupling basis is dubious.

Lastly, the arguments of Section 1.4 suggest that solving quantum field theory in the strong-coupling limit may be exceedingly difficult. It is perhaps overly optimistic to jump directly to this limit. I choose to work in the weak-coupling limit, where we understand things, and then see how far I can push the coupling constants.

The strong-coupling basis has been used by Kovarik *et al.* [KDK85, KDK86], but I choose not to use it for the reasons above.

2.2.4 Weak-Coupling Basis

The *weak-coupling basis*, also know as the Fock basis, is determined by the free particle number operators $\{a_{\mathbf{p}}^\dagger a_{\mathbf{p}}\}$. A basis state A is fixed by specifying the number $A_{\mathbf{p}}$ of free particles with momentum $\mathbf{p}$ for each $\mathbf{p}$. Since the field is a scalar, the particles are bosons, so each $A_{\mathbf{p}}$ can be any nonnegative integer. In particular, we can construct the state A by applying creation operators to the vacuum $|0;\mu\rangle$ for free particles of mass μ:

$$|A\rangle = \prod_{\mathbf{p}} (A_{\mathbf{p}}!)^{-1/2} (a_{\mathbf{p}}^\dagger)^{A_{\mathbf{p}}} |0;\mu\rangle. \tag{2.33}$$

Defined in this way the states are orthonormal:

$$\langle A|B\rangle = \delta_{A,B}. \tag{2.34}$$

When applied to the state A, the operator $a_{\mathbf{p}}^\dagger a_{\mathbf{p}}$ gives the number of particles with momentum $\mathbf{p}$, and the operators $a_{\mathbf{p}}$ and $a_{\mathbf{p}}^\dagger$ destroy or create one free particle with momentum $\mathbf{p}$, respectively:

$$a_{\mathbf{p}}^\dagger a_{\mathbf{p}} |A\rangle = A_{\mathbf{p}} |A\rangle, \tag{2.35}$$

$$a_{\mathbf{p}}|A\rangle = \sqrt{A_{\mathbf{p}}}|A'\rangle, \qquad \text{where } A'_{\mathbf{p}'} = \begin{cases} A_{\mathbf{p}} - 1, & \text{if } \mathbf{p}' = \mathbf{p}; \\ A_{\mathbf{p}}, & \text{otherwise,} \end{cases} \tag{2.36}$$

$$a_{\mathbf{p}}^\dagger|A\rangle = \sqrt{A_{\mathbf{p}} + 1}|A'\rangle, \qquad \text{where } A'_{\mathbf{p}'} = \begin{cases} A_{\mathbf{p}} + 1, & \text{if } \mathbf{p}' = \mathbf{p}; \\ A_{\mathbf{p}}, & \text{otherwise.} \end{cases} \tag{2.37}$$

In particular, we get zero when we apply $a_{\mathbf{p}}$ if $A_{\mathbf{p}} = 0$, that is when we try to destroy a nonexistent particle.

The weak-coupling basis is complete, and is amenable to numerical methods. Furthermore, basis states do possess definite total momentum P_i and parity R:

$$P_i|A\rangle = \left(\sum_{\mathbf{p}} A_{\mathbf{p}} p_i\right)|A\rangle, \tag{2.38}$$

$$R|A\rangle = (-1)^{\sum_{\mathbf{p}} A_{\mathbf{p}}}|A\rangle. \tag{2.39}$$

In other words, the total momentum of a state is the sum of the momenta of the particles in the state, and the parity of the state is even (odd) if the number of particles in the state is even (odd). Recall that momentum space is periodic, so the sum in the total momentum (2.38) must be interpreted mod $2\pi/a$.

In the case of zero coupling, that is a free theory, the weak-coupling basis states are, in fact, energy eigenstates, as can be seen from the hamiltonian (2.26c), so long as we choose $\frac{1}{2}\mu^2 = \lambda_2 = \frac{1}{2}m^2$. Thus we expect the basis to work well for weak coupling. Furthermore, since the basis depends on a nonlinear parameter μ, the mass of fictitious free particles, we might be able to adjust μ so that the basis works well for moderate or strong coupling. We expect weak-coupling basis states to reflect long-range behavior, since free particles of definite momentum are completely nonlocalized. Lastly, in Section 2.3 we see that all calculations with the weak-coupling basis can be done efficiently using only algebraic operations: No numerical integration nor numerical solution of differential equations is required. Thus for all these reasons, I choose to work with the weak-coupling basis.

2.3 Weak-Coupling Basis Calculations

In order to apply the variational methods of Chapter 1 to real scalar quantum field theory using the weak-coupling basis, we need to calculate hamiltonian matrix

elements between weak-coupling basis states. In addition, in order to estimate errors, we need to calculate the variance $(\Delta H)^2$ of each approximate energy eigenstate. In order to calculate physically significant quantities in quantum field theory, we need to calculate $\tilde{\phi}_{\mathbf{p}}$ matrix elements between (approximate) energy eigenstates, as we will see in Chapter 3. We may also be interested in calculating, say, $\langle \phi_{\mathbf{x}} \phi_{\mathbf{x}'} \rangle$ in the vacuum state. In this section I discuss the technical details of how to perform these calculations efficiently.

2.3.1 Calculation of Hamiltonian Matrix Elements

In this subsection I show how to calculate the matrix element $\langle B|H|A\rangle$. The key results are Equations (2.46b), (2.47) and (2.49).

We want to calculate $\langle B|H|A\rangle = \langle B|H_{\text{free}} + H_{\text{int}}|A\rangle$, where A and B are selected weak-coupling basis states. Recall from Equation (2.26c) that

$$H_{\text{free}} = \sum_{\mathbf{p}} \omega_{\mathbf{p}} \left(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + \tfrac{1}{2}\right), \tag{2.40}$$

$$H_{\text{int}} = \sum_{k=0}^{\infty} \lambda'_k \sum_{\mathbf{p}_1,\ldots,\mathbf{p}_k} \delta_{\mathbf{p}_1+\cdots+\mathbf{p}_k}\, \omega_{\mathbf{p}_1}^{-1/2} \cdots \omega_{\mathbf{p}_k}^{-1/2} (a_{\mathbf{p}_1} + a^\dagger_{-\mathbf{p}_1}) \cdots (a_{\mathbf{p}_k} + a^\dagger_{-\mathbf{p}_k}), \tag{2.41}$$

where I define

$$\lambda'_k = 2^{-k/2} \left(\lambda_k - \tfrac{1}{2}\mu^2 \delta_{k,2}\right) L^{(1-k/2)(d-1)}. \tag{2.42}$$

Note that $\langle B|H|A\rangle = 0$ unless A and B are in the same sector—that is have the same total momentum and, if the potential density $V(\phi)$ is even in ϕ, the same parity—as I assume in what follows.

Using the orthonormality condition (2.34) and the number operator rule (2.35), we see that

$$\langle B|H_{\text{free}}|A\rangle = \delta_{B,A} \sum_{\mathbf{p}} \omega_{\mathbf{p}} \left(A_{\mathbf{p}} + \tfrac{1}{2}\right). \tag{2.43}$$

But $\langle B|H_{\text{int}}|A\rangle$ is problematic. The λ'_k term allows us to go from A to B by destroying *or creating* any k particles, so long as the total momentum is unchanged.

For example, consider the λ'_6 term. Suppose the lattice has $N = 20$ points and that $A = B$. We can create 3 particles with arbitrary momenta $-\mathbf{p}_4$, $-\mathbf{p}_5$, $-\mathbf{p}_6$ and then destroy them by choosing $\mathbf{p}_1 = -\mathbf{p}_4$, $\mathbf{p}_2 = -\mathbf{p}_5$, $\mathbf{p}_3 = -\mathbf{p}_6$. Neglecting

symmetry factors of order unity, there are $20^3 = 8000$ ways to choose the 3 momenta. In other words, we have to add roughly 8000 terms to calculate just the λ'_6 term of just one matrix element! This is not computationally practical.

The problem is that we can create particles with arbitrary momenta. The solution is to normal order, that is to use the commutation relations (2.25) to put all destruction operators to the right of all creation operators: $a_{\mathbf{p}} a^\dagger_{\mathbf{p}'} = a^\dagger_{\mathbf{p}'} a_{\mathbf{p}} + \delta_{\mathbf{p},\mathbf{p}'}$. Then the destruction operators are constrained to destroy only particles in A and the creation operators, acting on the left, to destroy only particles in B. Typically, A and B each consist of only a few particles, thus the combinatorial possibilities are greatly reduced.

What follows is all combinatorics. The key observation is that for any pair of indices $\mathbf{p}_i, \mathbf{p}_j, 1 \le i < j \le k$, we need to commute $a_{\mathbf{p}_i}$ and $a^\dagger_{-\mathbf{p}_j}$ in the factors $(a_{\mathbf{p}_i} + a^\dagger_{-\mathbf{p}_i}) \cdots (a_{\mathbf{p}_j} + a^\dagger_{-\mathbf{p}_j})$. In doing so we get $(a_{\mathbf{p}_i} + a^\dagger_{-\mathbf{p}_i}) \cdots (a_{\mathbf{p}_j} + a^\dagger_{-\mathbf{p}_j})$, normal ordered, plus a "contraction" term $\delta_{\mathbf{p}_i+\mathbf{p}_j}$. If we do not contract the $\mathbf{p}_i$ and $\mathbf{p}_j$ factors, then they are each free to contract with other factors. If we do contract the $\mathbf{p}_i$ and $\mathbf{p}_j$ factors, then the Kronecker delta commutes with everything and no further contractions with the $\mathbf{p}_i$ or $\mathbf{p}_j$ factors are possible. In other words, when we normal order we get a term for each choice of zero or more disjoint pairs from the indices $\mathbf{p}_1, \ldots, \mathbf{p}_k$.

In particular,

$$\begin{aligned} H_{\text{int}} = \sum_{k=0}^{\infty} \lambda'_k \sum_{\ell=0}^{\lfloor k/2 \rfloor} & \frac{k!}{2^\ell \ell! (k-2\ell)!} \\ & \times \sum_{\mathbf{p}_1,\ldots,\mathbf{p}_{k-2\ell}} \sum_{\substack{\mathbf{r}_1,\ldots,\mathbf{r}_\ell \\ \mathbf{r}'_1,\ldots,\mathbf{r}'_\ell}} \delta_{\mathbf{p}_1+\cdots+\mathbf{p}_{k-2\ell}+\mathbf{r}_1+\mathbf{r}'_1+\cdots+\mathbf{r}_\ell+\mathbf{r}'_\ell} \\ & \quad \times \omega_{\mathbf{p}_1}^{-1/2} \cdots \omega_{\mathbf{p}_{k-2\ell}}^{-1/2} (\omega_{\mathbf{r}_1}\omega_{\mathbf{r}'_1})^{-1/2} \cdots (\omega_{\mathbf{r}_\ell}\omega_{\mathbf{r}'_\ell})^{-1/2} \\ & \quad\quad \times \delta_{\mathbf{r}_1,\mathbf{r}'_1} \cdots \delta_{\mathbf{r}_\ell,\mathbf{r}'_\ell} :(a_{\mathbf{p}_1} + a^\dagger_{-\mathbf{p}_1}) \cdots (a_{\mathbf{p}_{k-2\ell}} + a^\dagger_{-\mathbf{p}_{k-2\ell}}):. \end{aligned} \tag{2.44}$$

The combinatorial factor is the number of distinct ways to choose ℓ indistinguishable pairs, which I relabel $\{\mathbf{r}_1, \mathbf{r}'_1\}, \ldots, \{\mathbf{r}_\ell, \mathbf{r}'_\ell\}$, from the k indices $\mathbf{p}_1, \ldots, \mathbf{p}_k$, leaving $k-2\ell$ indices, which I relabel $\mathbf{p}_1, \ldots, \mathbf{p}_{k-2\ell}$. As usual, within the normal ordering symbols $:\cdots:$ all creation operators act to the left of all destruction operators, regardless of the order in which they appear.

We can eliminate the sums over $\mathbf{r}'_1, \ldots, \mathbf{r}'_\ell$ using Kronecker deltas, separate

out the sums over $\mathbf{r}_1, \ldots, \mathbf{r}_\ell$, and replace the sum over k by a sum over $k' = k - 2\ell$, which I relabel as k:

$$H_{\text{int}} = \sum_{k=0}^{\infty} \frac{1}{k!} \left[\sum_{\ell=0}^{\infty} \frac{(k+2\ell)!}{2^\ell \ell!} \lambda'_{k+2\ell} \left(\sum_{\mathbf{r}_1} \omega_{\mathbf{r}_1}^{-1} \right) \cdots \left(\sum_{\mathbf{r}_\ell} \omega_{\mathbf{r}_\ell}^{-1} \right) \right]$$
$$\times \sum_{\mathbf{p}_1, \ldots, \mathbf{p}_k} \delta_{\mathbf{p}_1 + \cdots + \mathbf{p}_k} \omega_{\mathbf{p}_1}^{-1/2} \cdots \omega_{\mathbf{p}_k}^{-1/2} :(a_{\mathbf{p}_1} + a^\dagger_{-\mathbf{p}_1}) \cdots (a_{\mathbf{p}_k} + a^\dagger_{-\mathbf{p}_k}): \tag{2.45a}$$
$$= \sum_{k=0}^{\infty} \frac{\hat{\lambda}_k}{k!} \sum_{\mathbf{p}_1, \ldots, \mathbf{p}_k} \delta_{\mathbf{p}_1 + \cdots + \mathbf{p}_k} \omega_{\mathbf{p}_1}^{-1/2} \cdots \omega_{\mathbf{p}_k}^{-1/2} :(a_{\mathbf{p}_1} + a^\dagger_{-\mathbf{p}_1}) \cdots (a_{\mathbf{p}_k} + a^\dagger_{-\mathbf{p}_k}):, \tag{2.45b}$$

where the normal ordered coupling constants are

$$\hat{\lambda}_k = \sum_{\ell=0}^{\infty} \frac{(k+2\ell)!}{2^\ell \ell!} \lambda'_{k+2\ell} \Omega^\ell \tag{2.46a}$$
$$= 2^{-k/2} L^{(1-k/2)(d-1)} \sum_{\ell=0}^{\infty} \frac{(k+2\ell)!}{4^\ell \ell!} \left(\lambda_{k+2\ell} - \tfrac{1}{2}\mu^2 \delta_{k+2\ell,2} \right) L^{-\ell(d-1)} \Omega^\ell, \tag{2.46b}$$

and I define

$$\Omega = \sum_{\mathbf{r}} \omega_{\mathbf{r}}^{-1}. \tag{2.47}$$

I have used the fact that $\omega_{\mathbf{r}'} = \omega_{-\mathbf{r}} = \omega_{\mathbf{r}}$. I keep the $k!$ factor in H_{int} separate for later convenience. Note that the normal ordered coupling constants depend on μ through λ'_2 and through ω in Ω.

It is convenient to introduce some mathematical language and notation. A state A is a *multiset* of particles with specified momenta. The concept of a multiset is a generalization of that of a set. A set either does not or does contain a particular element, that is it contains the element 0 or 1 times. A multiset may contain a particular element 0, 1 or more times, and these possibilities lead to distinct multisets. It is sometimes useful to generalize the concept of a multiset slightly by allowing a multiset to contain an element a negative number of times. In Table 2.3 I summarize various multiset notations.

Now that we have normal ordered H_{int}, Equation (2.45b), we want to calculate the matrix element $\langle B|H_{\text{int}}|A\rangle$, where A and B are basis states in the same sector. The destruction operators, acting on the right, destroy a multisubset A' of the particles in A, and the creation operators, acting on the left, destroy a multisubset B' of the particles in B. If the matrix element is nonzero, then the results of

Notation	Meaning
$A_{\mathbf{p}}$	The number of times the multiset A contains the element $\mathbf{p}$.
0	The null multiset: $0_{\mathbf{p}} = 0$ for all $\mathbf{p}$.
$A = B$	Multiset equality: $A_{\mathbf{p}} = B_{\mathbf{p}}$ for all $\mathbf{p}$.
$A \leq B$	Multiset inclusion: $A_{\mathbf{p}} \leq B_{\mathbf{p}}$ for all $\mathbf{p}$.
$A \subseteq B$	Set inclusion: $A_{\mathbf{p}} > 0$ implies $B_{\mathbf{p}} > 0$ for all $\mathbf{p}$.
$A + B$	Multiset sum: $(A+B)_{\mathbf{p}} = A_{\mathbf{p}} + B_{\mathbf{p}}$ for all $\mathbf{p}$.
$A - B$	Multiset difference: $(A-B)_{\mathbf{p}} = A_{\mathbf{p}} - B_{\mathbf{p}}$ for all $\mathbf{p}$.
nA	Multiset scalar product (n an integer): $(nA)_{\mathbf{p}} = n(A_{\mathbf{p}})$ for all $\mathbf{p}$.
$A \cup B$	Multiset union: $(A \cup B)_{\mathbf{p}} = \max(A_{\mathbf{p}}, B_{\mathbf{p}})$ for all $\mathbf{p}$.
$A \cap B$	Multiset intersection: $(A \cap B)_{\mathbf{p}} = \min(A_{\mathbf{p}}, B_{\mathbf{p}})$ for all $\mathbf{p}$.
$\#A$	Multiset cardinality (number of elements): $\#A = \sum_{\mathbf{p}} A_{\mathbf{p}}$.
$\lvert A \rvert$	Set cardinality (number of distinct elements): $\lvert A \rvert = \sum_{\mathbf{p}} \min(A_{\mathbf{p}}, 1)$.
$\overline{A}$	Multiset inversion: $\overline{A}_{\mathbf{p}} = A_{-\mathbf{p}}$.
$\sum A$	Multiset cummulation: $\sum A = \sum_{\mathbf{p}} A_{\mathbf{p}} \mathbf{p}$.

Table 2.3: Multiset notation.

destroying on the right and of destroying on the left must be the same *reduced state* $X = A - A' = B - B'$, which is virtual and need not be a selected state nor be in the same sector as A and B. The total number of particles destroyed going from A or B to X is $k = \#(A' + B')$.

What follows is more combinatorics. I want to write $\langle B|H_{\text{int}}|A\rangle$ as a sum over reduced states. We must match the indices $\mathbf{p}_1, \ldots, \mathbf{p}_k$ with the particles A' in A destroyed by $a_{\mathbf{p}}$'s and, distinctly, the particles B' in B destroyed by $a^\dagger_{-\mathbf{p}}$'s, where particles with the same momentum are indistinguishable. Then

$$\langle B|H_{\text{int}}|A\rangle = \sum_{\substack{A', B' \geq 0 \\ X = A - A' \\ = B - B' \geq 0}} \frac{\hat{\lambda}_{\#(A'+B')}}{\#(A'+B')!} \frac{\#(A'+B')!}{\prod_{\mathbf{p}} A'_{\mathbf{p}}! B'_{\mathbf{p}}!} \prod_{\mathbf{p}} \omega_{\mathbf{p}}^{-(A'_{\mathbf{p}} + B'_{\mathbf{p}})/2} \frac{\sqrt{A_{\mathbf{p}}! B_{\mathbf{p}}!}}{X_{\mathbf{p}}!}. \tag{2.48}$$

The second factor is combinatorial. The ω factor includes $\omega_{\mathbf{p}}^{-1/2}$ for each particle destroyed. The last factor follows from the destruction and creation operator rules

(2.36) and (2.37).

In summary, if A and B are in the same sector, then

$$\langle B|H|A\rangle = \delta_{B,A}\sum_{\mathbf{p}}\omega_{\mathbf{p}}\left(A_{\mathbf{p}}+\tfrac{1}{2}\right) + \sum_{\substack{A',B'\geq 0\\ X=A-A'\\ =B-B'\geq 0}}\hat{\lambda}_{\#(A'+B')}\prod_{\mathbf{p}}A'_{\mathbf{p}}!^{-1}B'_{\mathbf{p}}!^{-1}\,\omega_{\mathbf{p}}^{-(A'_{\mathbf{p}}+B'_{\mathbf{p}})/2}\,\frac{\sqrt{A_{\mathbf{p}}!B_{\mathbf{p}}!}}{X_{\mathbf{p}}!}. \quad (2.49)$$

Of course, if A and B are in different sectors, then $\langle B|H|A\rangle = 0$.

In practice, we first calculate Ω using Equation (2.47). Then we calculate the normal ordered coupling constants $\hat{\lambda}_k$ using Equation (2.46b). If the potential density $V(\phi)$ is a polynomial of degree r in ϕ, that is if the coupling constant $\lambda_k = 0$ unless $k \leq r$, then $\lambda'_k = \hat{\lambda}_k = 0$ unless $k \leq r$,[2] thus we need calculate only a finite number of $\hat{\lambda}_k$. Even if there are an infinite number of nonzero coupling constants, we need calculate $\hat{\lambda}_k$ for only $k \leq 2\#A$, where A is a selected basis state with the largest number of particles, since the normal ordered hamiltonian can only destroy particles. But if there are an infinite number of nonzero coupling constants, then each $\hat{\lambda}_k$ is the sum of an infinite number of terms, which we anticipate converges, and hence can be truncated.

Finally, using Equation (2.49) we calculate $\langle B|H|A\rangle$ for each of the n^2 choices of selected basis states A and B. The time to compute one matrix element is $O(1)$, if the potential density $V(\phi)$ is a polynomial in ϕ, and no more than $O(n)$, if $V(\phi)$ is an infinite power series in ϕ.[3] Thus the time to compute all n^2 matrix elements is no more than $O(n^3)$, the time to diagonalize the matrix. Thus we can efficiently calculate hamiltonian matrix elements between weak-coupling basis states.

2.3.2 Calculation of Variances

In this subsection I show how to calculate the variance $(\Delta H)^2$ of an approximate eigenstate provided by the Rayleigh-Ritz method. Doing so involves special

[2]This is not strictly true if $r \leq 2$.

[3]The latter statement is false if the basis is pathologically *sparse*, for example, if the n basis states consist of $n, 2n, \ldots, n^2$ particles, respectively.

difficulties. The key results are Equations (2.56), (2.63), (2.64), (2.65), (2.66) and (2.67).

If v is any state, then

$$(\Delta H)_v^2 = \langle v|(H-\langle H\rangle)^2|v\rangle = \langle v|H^2|v\rangle - \langle v|H|v\rangle^2. \quad (2.50)$$

Unfortunately, the last expression is not useful for numerical methods: It expresses the variance, which we hope is small, as the difference of two large quantities, providing little or no accuracy.

But suppose v is in the n-dimensional subspace $\mathcal{V}_n$ of Hilbert space spanned by the selected basis states $u_1, \ldots, u_n$. Recall that $P_n = \sum_{i=1}^n |u_i\rangle\langle u_i|$ is the orthogonal projection operator onto $\mathcal{V}_n$ and $P'_n = \sum_{i=n+1} |u_i\rangle\langle u_i|$ is the orthogonal projection operator onto $\mathcal{V}_n^\perp$. Then $P_n|v\rangle = |v\rangle$. If we insert $1_\mathcal{V} = P_n + P'_n$ into H^2, then (Figure 1.1)

$$(\Delta H)^2 = \underbrace{\langle v|P_nHP_n\,P_nHP_n|v\rangle - \langle v|P_nHP_n|v\rangle^2}_{\text{intrinsic variance}} + \underbrace{\langle v|P_nHP'_n\,P'_nHP_n|v\rangle}_{\text{extrinsic variance}}. \quad (2.51)$$

The variance is the sum of the *intrinsic variance* and the *extrinsic variance* relative to $\mathcal{V}_n$, which are both nonnegative. The intrinsic variance is the variance of $H_n = P_nHP_n$ and is calculated "entirely within" $\mathcal{V}_n$. The extrinsic variance "goes outside of" $\mathcal{V}_n$, and can be calculated by summing over intermediate unselected basis states:

$$(\Delta H)_{\text{ext}}^2 = \langle v|HP'_nH|v\rangle = \sum_{i=n+1}\langle v|H|u_i\rangle\langle u_i|H|v\rangle. \quad (2.52)$$

The loss of accuracy in the variance results entirely from the intrinsic variance, which is the difference of two large quantities: There is no loss of accuracy when calculating the extrinsic variance.

Since H_{free} is diagonal in the weak-coupling basis, it does not connect selected and unselected basis states. Thus we can use H_{int} in place of H in the expression above, when using the weak-coupling basis.

If v is an eigenstate of H_n, for example, one provided by the Rayleigh-Ritz method, then the intrinsic variance is zero. In this case, the variance is simply the extrinsic variance and we can calculate it using Equation (2.52). Unfortunately, this

expression is a sum over, in general, many unselected basis states, each connected to at least one selected basis state by $H_{\rm int}$.

For example, consider again a hamiltonian with a ϕ^6 term. Suppose the lattice has $N = 20$ points and the only selected basis state is the free particle vacuum. The ϕ^6 term destroys or creates 6 free particles. If we choose $\mathbf{p}_1, \ldots, \mathbf{p}_5$ arbitrarily and $\mathbf{p}_6 = -\mathbf{p}_1 - \cdots - \mathbf{p}_5$, then the ϕ^6 term connects the free particle vacuum to the state $|\mathbf{p}_1, \ldots, \mathbf{p}_6\rangle$. Neglecting symmetry factors of order unity, there are $20^5 = 3.2 \times 10^6$ ways to choose 5 such momenta. Thus if we use Equation (2.52) to calculate the extrinsic variance, we need to add roughly 3.2×10^6 terms! This is not computationally practical.

As we saw before, if we normal order, we avoid creating particles with arbitrary momenta and thus can calculate efficiently. The trick is to combine normal ordering with the extrinsic variance so that we can calculate efficiently without loss of accuracy.

Thus we want to normal order $H^2_{\rm int}$. I start with $H_{\rm int}$ in normal ordered form, Equation (2.45b). Then

$$\begin{aligned} H^2_{\rm int} = & \sum_{k=0}^{\infty} \frac{\hat\lambda_k}{k!} \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_k} \delta_{\mathbf{q}_1+\cdots+\mathbf{q}_k}\, \omega_{\mathbf{q}_1}^{-1/2} \cdots \omega_{\mathbf{q}_k}^{-1/2} :(a_{\mathbf{q}_1}+a^\dagger_{-\mathbf{q}_1}) \cdots (a_{\mathbf{q}_k}+a^\dagger_{-\mathbf{q}_k}): \\ & \times \sum_{j=0}^{\infty} \frac{\hat\lambda_j}{j!} \sum_{\mathbf{p}_1,\ldots,\mathbf{p}_j} \delta_{\mathbf{p}_1+\cdots+\mathbf{p}_j}\, \omega_{\mathbf{p}_1}^{-1/2} \cdots \omega_{\mathbf{p}_j}^{-1/2} :(a_{\mathbf{p}_1}+a^\dagger_{-\mathbf{p}_1}) \cdots (a_{\mathbf{p}_j}+a^\dagger_{-\mathbf{p}_j}):. \end{aligned} \tag{2.53}$$

As with $H_{\rm int}$ before, when we normal order we get a term for each choice of zero or more contraction pairs from the indices $\mathbf{p}_1, \ldots, \mathbf{p}_j, \mathbf{q}_1, \ldots, \mathbf{q}_k$. But since each $H_{\rm int}$ is already separately normal ordered, each pair must have one index from $\mathbf{p}_1, \ldots, \mathbf{p}_j$ and one from $\mathbf{q}_1, \ldots, \mathbf{q}_k$. Thus

$$\begin{aligned} H^2_{\rm int} = & \sum_{j,k=0}^{\infty} \frac{\hat\lambda_j}{j!} \frac{\hat\lambda_k}{k!} \sum_{\ell=0}^{\min(j,k)} \frac{j!k!}{\ell!(j-\ell)!(k-\ell)!} \\ & \times \sum_{\substack{\mathbf{p}_1,\ldots,\mathbf{p}_{j-\ell} \\ \mathbf{q}_1,\ldots,\mathbf{q}_{k-\ell}}} \sum_{\substack{\mathbf{r}_1,\ldots,\mathbf{r}_\ell \\ \mathbf{r}'_1,\ldots,\mathbf{r}'_\ell}} \delta_{\mathbf{p}_1+\cdots+\mathbf{p}_{j-\ell}+\mathbf{q}_1+\cdots+\mathbf{q}_{k-\ell}+\mathbf{r}_1+\cdots+\mathbf{r}_\ell+\mathbf{r}'_1+\cdots+\mathbf{r}'_\ell}\, \delta_{\mathbf{p}_1+\cdots+\mathbf{p}_{j-\ell}+\mathbf{r}'_1+\cdots+\mathbf{r}'_\ell} \\ & \times \omega_{\mathbf{p}_1}^{-1/2} \cdots \omega_{\mathbf{p}_{j-\ell}}^{-1/2} \omega_{\mathbf{q}_1}^{-1/2} \cdots \omega_{\mathbf{q}_{k-\ell}}^{-1/2} (\omega_{\mathbf{r}_1}\omega_{\mathbf{r}'_1})^{-1/2} \cdots (\omega_{\mathbf{r}_\ell}\omega_{\mathbf{r}'_\ell})^{-1/2}\, \delta_{\mathbf{r}_1+\mathbf{r}'_1} \cdots \delta_{\mathbf{r}_\ell+\mathbf{r}'_\ell} \\ & \times :(a_{\mathbf{p}_1}+a^\dagger_{-\mathbf{p}_1}) \cdots (a_{\mathbf{p}_{j-\ell}}+a^\dagger_{-\mathbf{p}_{j-\ell}})(a_{\mathbf{q}_1}+a^\dagger_{-\mathbf{q}_1}) \cdots (a_{\mathbf{q}_{k-\ell}}+a^\dagger_{-\mathbf{q}_{k-\ell}}):. \end{aligned} \tag{2.54}$$

The first Kronecker delta, expressing total momentum conservation, results from combining the two Kronecker deltas in the previous expression. The combinatorial factor is the number of distinct ways to choose ℓ indistinguishable pairs, which I relabel $\{\mathbf{r}_1, \mathbf{r}'_1\}, \ldots, \{\mathbf{r}_\ell, \mathbf{r}'_\ell\}$. The ℓ indices $\mathbf{r}'_1, \ldots, \mathbf{r}'_\ell$ are chosen from the j indices $\mathbf{p}_1, \ldots, \mathbf{p}_j$, leaving $j - \ell$ indices, which I relabel $\mathbf{p}_1, \ldots, \mathbf{p}_{j-\ell}$. Likewise, the ℓ indices $\mathbf{r}_1, \ldots, \mathbf{r}_\ell$ are chosen from the k indices $\mathbf{q}_1, \ldots, \mathbf{q}_k$, leaving $k-\ell$ indices, which I relabel $\mathbf{q}_1, \ldots, \mathbf{q}_{k-\ell}$.

We can eliminate the sums over $\mathbf{r}'_1, \ldots, \mathbf{r}'_\ell$ using Kronecker deltas, and replace the sums over j and k by sums over $j' = j - \ell$ and $k' = k - \ell$, which I relabel as j and k, respectively:

$$\begin{aligned} H^2_{\rm int} = & \sum_{j,k=0}^{\infty} \frac{1}{j!k!} \sum_{\substack{\mathbf{p}_1,\ldots,\mathbf{p}_j \\ \mathbf{q}_1,\ldots,\mathbf{q}_k}} \delta_{\mathbf{p}_1+\cdots+\mathbf{p}_j+\mathbf{q}_1+\cdots+\mathbf{q}_k} \\ & \times \left\{ \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \hat\lambda_{j+\ell} \hat\lambda_{k+\ell} \left[\sum_{\mathbf{r}_1,\ldots,\mathbf{r}_\ell} \delta_{\mathbf{p}_1+\cdots+\mathbf{p}_j-\mathbf{r}_1-\cdots-\mathbf{r}_\ell}\, \omega_{\mathbf{r}_1}^{-1} \cdots \omega_{\mathbf{r}_\ell}^{-1} \right] \right\} \\ & \times \omega_{\mathbf{p}_1}^{-1/2} \cdots \omega_{\mathbf{p}_j}^{-1/2} \omega_{\mathbf{q}_1}^{-1/2} \cdots \omega_{\mathbf{q}_k}^{-1/2} \\ & \times :(a_{\mathbf{p}_1}+a^\dagger_{-\mathbf{p}_1}) \cdots (a_{\mathbf{p}_j}+a^\dagger_{-\mathbf{p}_j})(a_{\mathbf{q}_1}+a^\dagger_{-\mathbf{q}_1}) \cdots (a_{\mathbf{q}_k}+a^\dagger_{-\mathbf{q}_k}): \end{aligned} \tag{2.55a}$$

$$\begin{aligned} = & \sum_{j,k=0}^{\infty} \frac{1}{j!k!} \sum_{\substack{\mathbf{p}_1,\ldots,\mathbf{p}_j \\ \mathbf{q}_1,\ldots,\mathbf{q}_k}} \delta_{\mathbf{p}_1+\cdots+\mathbf{p}_j+\mathbf{q}_1+\cdots+\mathbf{q}_k}\, \hat\lambda_{j,k}(\mathbf{p}_1+\cdots+\mathbf{p}_j) \\ & \times \omega_{\mathbf{p}_1}^{-1/2} \cdots \omega_{\mathbf{p}_j}^{-1/2} \omega_{\mathbf{q}_1}^{-1/2} \cdots \omega_{\mathbf{q}_k}^{-1/2} \\ & \times :(a_{\mathbf{p}_1}+a^\dagger_{-\mathbf{p}_1}) \cdots (a_{\mathbf{p}_j}+a^\dagger_{-\mathbf{p}_j})(a_{\mathbf{q}_1}+a^\dagger_{-\mathbf{q}_1}) \cdots (a_{\mathbf{q}_k}+a^\dagger_{-\mathbf{q}_k}):, \end{aligned} \tag{2.55b}$$

where the normal ordered coupling functions for $H^2_{\rm int}$ are

$$\hat\lambda_{j,k}(\mathbf{p}) = \sum_{\ell=0}^{\infty} \hat\lambda_{j+\ell} \hat\lambda_{k+\ell}\, \Omega_\ell(\mathbf{p}), \tag{2.56}$$

and I define

$$\Omega_\ell(\mathbf{p}) = \frac{1}{\ell!} \sum_{\mathbf{r}_1,\ldots,\mathbf{r}_\ell} \delta_{\mathbf{p},\mathbf{r}_1+\cdots+\mathbf{r}_\ell}\, \omega_{\mathbf{r}_1}^{-1} \cdots \omega_{\mathbf{r}_\ell}^{-1}. \tag{2.57}$$

I keep the $j!$ and $k!$ factors in $H^2_{\rm int}$ separate for later convenience.

Now that we have normal ordered $H^2_{\rm int}$, Equation (2.55b), we want to calculate $\langle B|H^2_{\rm int}|A\rangle$, where A and B are selected basis states in the same sector. I continue

much as I did for hamiltonian matrix elements. Since $H^2_{\rm int}$ is normal ordered, destruction operators, acting on the right, destroy particles in A and creation operators, acting on the left, destroy particles in B. But the p's and q's are distinct, since the argument of the normal ordered coupling function $\hat\lambda_{j,k}$ involves only the p's. Thus we choose multisubsets A', A'' of particles in A destroyed by $a_{\rm p}$'s and $a_{\rm q}$'s, respectively, and multisubsets B', B'' of particles in B destroyed by $a^\dagger_{-\rm q}$'s and $a^\dagger_{-\rm p}$'s, respectively. If the matrix element is nonzero, then the results of destroying on the right and destroying on the left must be the same reduced state $X = A - A' - A'' = B - B' - B''$, which is virtual and need not be a selected state nor in the same sector as A and B.

What follows is more combinatorics. I want to write $\langle B|H^2_{\rm int}|A\rangle$ as a sum over reduced states. We must match the indices $\rm p_1,\ldots,p_j$ with particles in A' and B'', and the indices $\rm q_1,\ldots,q_k$ with particles in B' and A'', where particles with the same momentum are indistinguishable. Then

$$\begin{aligned}\langle B|H^2_{\rm int}|A\rangle &= \sum_{\substack{A',A'',B',B''\ge 0\\ X=A-A'-A''\\ =B-B'-B''\ge 0}} \frac{\hat\lambda_{\#(A'+B''),\#(B'+A'')}(\sum A'+\overline{B''})}{\#(A'+B'')!\#(B'+A'')!}\,\frac{\#(A'+B'')!}{\prod_{\rm p} A'_{\rm p}!B''_{\rm p}!}\,\frac{\#(B'+A'')!}{\prod_{\rm p} B'_{\rm p}!A''_{\rm p}!}\\ &\qquad\times\prod_{\rm p}\omega_{\rm p}^{-(A'_{\rm p}+A''_{\rm p}+B'_{\rm p}+B''_{\rm p})/2}\,\frac{\sqrt{A_{\rm p}!B_{\rm p}!}}{X_{\rm p}!} \qquad (2.58a)\\ &= \sum_{\substack{A',A'',B',B''\ge 0\\ X=A-A'-A''\\ =B-B'-B''\ge 0}} \hat\lambda_{\#(A'+B''),\#(B'+A'')}(\sum A'+\overline{B''})\\ &\qquad\times\prod_{\rm p} A'_{\rm p}!^{-1}A''_{\rm p}!^{-1}B'_{\rm p}!^{-1}B''_{\rm p}!^{-1}\,\omega_{\rm p}^{-(A'_{\rm p}+A''_{\rm p}+B'_{\rm p}+B''_{\rm p})/2}\,\frac{\sqrt{A_{\rm p}!B_{\rm p}!}}{X_{\rm p}!}. \qquad (2.58b)\end{aligned}$$

In the momentum argument of $\hat\lambda_{j,k}$, the multiset B'' is inverted, because these are particles destroyed by $a^\dagger_{-\rm p}$'s but we want the sum of the p's. The second and third factors in the first expression are combinatorial. The ω factor includes $\omega_{\rm p}^{-1/2}$ for each particle destroyed. The last factor follows from the destruction and creation operator rules (2.36) and (2.37).

But what we really want to calculate is

$$\langle B|H_{\rm int}P'_nH_{\rm int}|A\rangle = \langle B|H^2_{\rm int}|A\rangle - \sum_{C\ \text{selected}}\langle B|H_{\rm int}|C\rangle\langle C|H_{\rm int}|A\rangle. \qquad (2.59)$$

Here C is a selected basis state in the same sector as A and B. We can calculate

$\langle B|H_{\rm int}P'_nH_{\rm int}|A\rangle$ by identifying the intermediate state C in the derivation of Equation (2.58b) for $\langle B|H^2_{\rm int}|A\rangle$ and excluding terms such that C is selected.

Consider $\hat\lambda_{j,k}(\rm p)$, which is the expression in curly braces in Equation (2.55a) for $H^2_{\rm int}$. I want to rewrite the sums over $\rm r_1,\ldots,r_\ell$ as a sum over multisets $C' = \{\rm r_1,\ldots,r_\ell\}$. We must match the indices $\rm r_1,\ldots,r_\ell$ with the particles in C', where particles with the same momentum are indistinguishable. Then

$$\begin{aligned}\hat\lambda_{j,k}(\rm p) &= \sum_{\ell=0}^{\infty}\frac{1}{\ell!}\hat\lambda_{j+\ell}\hat\lambda_{k+\ell}\sum_{\substack{C'\\ \#C'=\ell\\ \sum C'=\rm p}}\frac{\#(C')!}{\prod_{\rm r}C'_{\rm r}!}\prod_{\rm r}\omega_{\rm r}^{-C'_{\rm r}} \qquad (2.60a)\\ &= \sum_{\ell=0}^{\infty}\hat\lambda_{j+\ell}\hat\lambda_{k+\ell}\sum_{\substack{C'\\ \#C'=\ell\\ \sum C'=\rm p}}\prod_{\rm r}C'_{\rm r}!^{-1}\,\omega_{\rm r}^{-C'_{\rm r}}. \qquad (2.60b)\end{aligned}$$

The second to last factor in the first expression is combinatorial.

Thus we can rewrite Equation (2.58b):

$$\begin{aligned}\langle B|H^2_{\rm int}|A\rangle = \sum_{\substack{A',A'',B',B''\ge 0\\ X=A-A'-A''\\ =B-B'-B''\ge 0}}&\left[\sum_{\ell=0}^{\infty}\hat\lambda_{\#(A'+B'')+\ell}\hat\lambda_{\#(B'+A'')+\ell}\sum_{\substack{C'\\ \#C'=\ell\\ \sum A'+\overline{B''}+\overline{C'}=0}}\prod_{\rm r}C'_{\rm r}!^{-1}\,\omega_{\rm r}^{-C'_{\rm r}}\right]\\ &\times\prod_{\rm p}A'_{\rm p}!^{-1}A''_{\rm p}!^{-1}B'_{\rm p}!^{-1}B''_{\rm p}!^{-1}\,\omega_{\rm p}^{-(A'_{\rm p}+A''_{\rm p}+B'_{\rm p}+B''_{\rm p})/2}. \qquad (2.61)\end{aligned}$$

Consider a single term specified by a choice of A', A'', B', B'', C'. The particles in A' correspond to $a_{\rm p}$'s, in A'' to $a_{\rm q}$'s, in B' to $a^\dagger_{-\rm q}$'s and in B'' to $a^\dagger_{-\rm p}$'s. The particles in C' correspond to $\delta_{\rm r+r'}$ factors in Equation (2.54) for $H^2_{\rm int}$ after normal ordering, which were $a_{\rm r}\cdots a^\dagger_{-\rm r'}$ $(= a_{\rm q}\cdots a^\dagger_{-\rm p})$ contraction pairs in Equation (2.53) for $H^2_{\rm int}$ before normal ordering. Thus before normal ordering the term under consideration was, schematically,

$$\langle B|\underbrace{a^\dagger_{-\rm q}}_{B'}\underbrace{a_{\rm q}}_{A''}\underbrace{a_{\rm r}}_{C'}|C\rangle\langle C|\underbrace{a^\dagger_{-\rm r'}}_{C'}\underbrace{a^\dagger_{-\rm p}}_{B''}\underbrace{a_{\rm p}}_{A'}|A\rangle, \qquad (2.62)$$

where the multisets indicate which particles are being destroyed or created by the corresponding operators. Thus the desired intermediate state is $C = A - A' + B'' + C' = B - B' + A'' + C'$. Note that $C \ge Y$, where the *expanded state* $Y = A - A' + B'' =$

$B - B' + A''$, which is virtual and need not be a selected state nor in the same sector as A and B.

Then subtracting out undesired terms corresponding to selected C,

$$\begin{aligned}
&\langle B|H_{\rm int}P_n'H_{\rm int}|A\rangle \\
&= \sum_{\substack{A',A'',B',B''\geq 0\\ X=A-A'-A''\\ =B-B'-B''\geq 0}} [\hat\lambda_{\#(A'+B''),\#(B'+A'')}(\textstyle\sum A' + \overline{B''}) - \tilde\lambda_{\#(A'+B''),\#(B'+A'')}(A - A' + B'')] \\
&\qquad \times \prod_{\mathbf{p}} A_{\mathbf{p}}'!^{-1} A_{\mathbf{p}}''!^{-1} B_{\mathbf{p}}'!^{-1} B_{\mathbf{p}}''!^{-1}\, \omega_{\mathbf{p}}^{-(A_{\mathbf{p}}'+A_{\mathbf{p}}''+B_{\mathbf{p}}'+B_{\mathbf{p}}'')/2},
\end{aligned} \tag{2.63}$$

where I define correction functions to $\hat\lambda_{j,k}(\mathbf{p})$,

$$\tilde\lambda_{j,k}(Y) = \sum_{\ell=0}^{\infty} \hat\lambda_{j+\ell}\hat\lambda_{k+\ell}\,\Omega_\ell(Y), \tag{2.64}$$

and correction functions to $\Omega_\ell(\mathbf{p})$,

$$\tilde\Omega_\ell(Y) = \sum_{\substack{C'\\ \#C'=\ell\\ Y+C' \text{ selected}}} \prod_{\mathbf{r}} C_{\mathbf{r}}'!^{-1}\,\omega_{\mathbf{r}}^{-C_{\mathbf{r}}'}. \tag{2.65}$$

Finally, suppose v is a state in $\mathcal{V}_n$ that is an eigenstate of H_n, for example, an approximate energy eigenstate provided by the Rayleigh-Ritz method. Then

$$(\Delta H)_v^2 = \langle v|H_{\rm int}P_n'H_{\rm int}|v\rangle = \sum_{A,B} \langle v|B\rangle\langle B|H_{\rm int}P_n'H_{\rm int}|A\rangle\langle A|v\rangle. \tag{2.66}$$

In practice, we first calculate the $\Omega_\ell(\mathbf{p})$ using Equation (2.57). Note that $\Omega_0(\mathbf{p}) = \delta_{\mathbf{p}}$ and $\Omega_1(\mathbf{p}) = \omega_{\mathbf{p}}^{-1}$. We can calculate higher-order $\Omega_\ell(\mathbf{p})$ recursively:

$$\Omega_{\ell+1}(\mathbf{p}) = \sum_{\mathbf{r}_{\ell+1}} \sum_{\mathbf{r}_1,\ldots,\mathbf{r}_\ell} \delta_{\mathbf{p},\mathbf{r}_1+\cdots+\mathbf{r}_\ell+\mathbf{r}_{\ell+1}}\, \omega_{\mathbf{r}_1}^{-1}\cdots\omega_{\mathbf{r}_\ell}^{-1}\omega_{\mathbf{r}_{\ell+1}}^{-1} \tag{2.67a}$$

$$= \sum_{\mathbf{r}_{\ell+1}} \Omega_\ell(\mathbf{p}-\mathbf{r}_{\ell+1})\omega_{\mathbf{r}_{\ell+1}}^{-1}. \tag{2.67b}$$

Thus the $\Omega_\ell(\mathbf{p})$ can be calculated efficiently.

Then we calculate the normal ordered coupling functions $\hat\lambda_{j,k}(\mathbf{p})$ using Equation (2.56). If the potential density $V(\phi)$ is a polynomial of degree r in ϕ, then $\hat\lambda_k = 0$

unless $k \leq r$. Hence $\hat\lambda_{j,k}(\mathbf{p}) = 0$ unless $j, k \leq r$. Thus we need calculate only a finite number of $\hat\lambda_{j,k}(\mathbf{p})$ and $\Omega_\ell(\mathbf{p})$. Even if there are an infinite number of nonzero coupling constants, we need calculate $\hat\lambda_{j,k}(\mathbf{p})$ for only $j + k \leq 2\#A$, where A is a selected basis state with the largest number of particles, since a normal ordered operator can only destroy particles. But if there are an infinite number of nonzero coupling constants, then each $\hat\lambda_{j,k}(\mathbf{p})$ is the sum of an infinite number of terms involving $\Omega_\ell(\mathbf{p})$ for arbitrarily large ℓ. But we anticipate that the series for each $\hat\lambda_{j,k}(\mathbf{p})$ converges, and hence can be truncated.

Then we calculate the correction functions $\tilde\Omega_\ell(Y)$ using Equation (2.65). Note that $\tilde\Omega_\ell(C) = 0$ for all $\ell > \#(C-Y)$, where C is a selected basis state containing Y ($C \geq Y$) with the largest number of particles. Then we calculate the correction functions $\tilde\lambda_{j,k}(Y)$ using Equation (2.64) for the same finite set of values of j, k as for $\hat\lambda_{j,k}(\mathbf{p})$. Each $\tilde\lambda_{j,k}(Y)$ is a finite sum, since high-order $\tilde\Omega_\ell(Y)$ are zero. Thus we can calculate the correction functions effectively.

The correction functions are needed for each expanded state $Y \leq C$ for at least one selected basis state C. If the set of selected basis states is *compact*—that is if all multisubsets of a selected basis state that are in the same sector are also selected—or approximately compact, then the number of such Y is $O(n)$, where n is the number of selected basis states. The number of terms in $\tilde\Omega_\ell(Y)$ or in $\tilde\lambda_{j,k}(Y)$ is no more than $O(n)$, thus the time to compute all the correction functions is no more than $O(n^2)$. In Appendix A I discuss how to compute the correction functions efficiently.

Then we calculate $\langle B|H_{\rm int}P_n'H_{\rm int}|A\rangle$ using Equation (2.63) for each of the n^2 choices of selected basis states A and B. The time to compute one matrix element is $O(1)$, if the potential density $V(\phi)$ is a polynomial in ϕ, and no more than $O(n)$, if $V(\phi)$ is an infinite power series in ϕ. Thus the time to compute all n^2 matrix elements is no more than $O(n^3)$, the time to diagonalize the matrix.

Finally, we calculate the variance for each of the n approximate energy eigenstates using Equation (2.66). The time to compute each variance is $O(n^2)$, thus the time to compute all variances is $O(n^3)$

In summary, we can efficiently calculate the variances of all approximate energy eigenstates in $O(n^3)$ time.

2.3.3 Calculation of Other Interesting Quantities

In order to calculate physically significant quantities in quantum field theory, we need to compute $\tilde{\phi}_{\mathbf{p}}$ matrix elements between (approximate) energy eigenstates, as we will see in Chapter 3.

Suppose v_1 is a state—not necessarily an energy eigenstate—in some sector, that is v_1 has definite total momentum $\mathbf{p}_1$ and, if the potential density $V(\phi)$ is even in ϕ, definite parity. Then $|v_1\rangle = \sum_{A_1} |A_1\rangle\langle A_1|v_1\rangle$, where the sum is over the n_1 selected basis states for the sector. Similarly, suppose v_2 is a state in some, possibly different, sector with definite momentum $\mathbf{p}_2$. Then $|v_2\rangle = \sum_{A_2} |A_2\rangle\langle A_2|v_2\rangle$, where the sum is over the n_2 selected basis states for the sector. Thus

$$\langle v_2|\tilde{\phi}_{\mathbf{p}}|v_1\rangle = \sum_{A_1,A_2} \langle v_2|A_2\rangle\langle A_2|\tilde{\phi}_{\mathbf{p}}|A_1\rangle\langle A_1|v_1\rangle. \tag{2.68}$$

From Equation (2.18) we see that $\tilde{\phi}_{\mathbf{p}}$ destroys one free particle with momentum $\mathbf{p}$ or creates one free particle with momentum $-\mathbf{p}$. Hence the matrix element is zero unless $\mathbf{p}_1 - \mathbf{p}_2 = \mathbf{p}$. Furthermore, if the potential density $V(\phi)$ is even in ϕ, then the matrix element is zero unless v_1 and v_2 have opposite parity. Lastly, since $\tilde{\phi}_{\mathbf{p}}$ connects each basis state A_1 to at most two basis states A_2, the double sum is essentially a single sum. Thus the time to compute $\langle v_2|\tilde{\phi}_{\mathbf{p}}|v_1\rangle$ is $O(n) = O(\min(n_1, n_2))$.

We might be interested in calculating quantities other than those I have discussed above. Any quantity in quantum theory can be related to matrix elements of operators between states. Any operator can be expressed in terms of $\phi_{\mathbf{x}}$ and $\pi_{\mathbf{x}}$, or alternatively in terms of $a_{\mathbf{p}}$ and $a^\dagger_{-\mathbf{p}}$. Any state can be expressed as a linear combination of weak-coupling basis states. Thus we can calculate any matrix element using only algebraic operations. Of course, as we have seen above, normal ordering and other tricks are useful for increasing computational efficiency.

Here we come to the end of a long, technical chapter. I have introduced real scalar field theories on finite lattices, to which I apply my method. I have discussed various choices of bases and argued for one: the weak-coupling basis. Finally, I have shown how we can efficiently calculate quantities necessary to my method using the weak-coupling basis.

As I discussed at the end of Section 2.1, we can take either of two viewpoints.

First, we can interpret our theory as describing a set of coupled oscillators, unrelated to any quantum field theory. We now have all the tools necessary for this viewpoint, which I take up in Appendix B. Second, we can interpret our theory on a finite lattice as an approximation to an infinite-volume, continuum quantum field theory. I develop this viewpoint in Chapter 3.

Chapter 3

Extending the Method to Quantum Field Theory

In Section 2.1 I introduced real scalar quantum field theories on a finite lattice. There are two related issues we must resolve before we can interpret finite-volume, lattice theories as approximations to corresponding infinite-volume, continuum theories. First, we must determine what theory we are approximating: The coupling constants $\lambda_\phi, \lambda_0, \lambda_1, \ldots$ are not *physical* coupling constants but *bare* coupling constants, which depend on the lattice size L and spacing a, as well as on the theory being approximated. Second, we must relate quantities we can calculate—energy eigenvalues, energy eigenstates and matrix elements between energy eigenstates—to physically interesting quantities—bound state energies and scattering amplitudes.

Some researchers [KDK86, DHK87, Dun87] side-step these issues and merely attempt to show that bare coupling constants and the lowest few bound state energies exhibit certain scaling behavior. Other researchers [BG80, Ste85, Ing86, Rit90] use the effective potential to address both issues. It is also possible to relate bound state energies to the long-range behavior of the two-point correlation function in the vacuum state, as is done in lattice gauge theory; but it is difficult to recognize the long-range behavior, unless one works on a very large lattice.

My approach to both issues is to relate Green's functions, which are physically significant, to energy eigenvalues, energy eigenstates and matrix elements between energy eigenstates. The values of Green's functions at special points are simply

related to physical coupling constants; the locations of poles in the two-point Green's function correspond to bound state energies; and Green's functions are simply related to scattering amplitudes. Thus by calculating Green's functions, we both determine what theory we are approximating and obtain physically interesting quantities. Although my approach is direct, surprisingly, it has not been used before, to the best of my knowledge.

I want to argue for my approach with a simple counting argument. Suppose Hilbert space has finite dimension n. The hamiltonian H is an $n \times n$ hermitian matrix. It is fixed by specifying $2n^2$ real quantities (n^2 complex quantities), which satisfy n^2 real conditions ($H^\dagger = H$). Thus H is fixed by specifying n^2 independent real quantities. The n energy eigenstates $\{e_i\}$ are fixed by specifying $2n^2$ real quantities, which satisfy n^2 real conditions ($\langle e_i | e_j \rangle = \delta_{ij}$) and include n insignificant phase factors, one for each eigenstate. Thus the n energy eigenstates $\{e_i\}$ together with the n energy eigenvalues $\{\varepsilon_i\}$ are fixed by specifying n^2 independent real quantities. Finally, the scattering matrix S is an $n \times n$ unitary matrix ($S^\dagger S = 1_V$), which is fixed by specifying n^2 independent real quantities.

In other words, the hamiltonian H, the collection of energy eigenvalues $\{\varepsilon_i\}$ and energy eigenstates $\{e_i\}$, and the scattering matrix S each represent the same amount of information, n^2 real quantities:

$$H \longleftrightarrow \{\varepsilon_i\}, \{e_i\} \longleftrightarrow S \tag{3.1}$$

The hamiltonian represents the theory and the scattering matrix summarizes the results of all possible experiments. The basic problem in particle physics is to relate H and S, theory and experiment. In Chapters 1 and 2 I showed how to calculate approximations to $\{\varepsilon_i\}$ and $\{e_i\}$ from H. In this chapter I complete the link and show how to calculate S from $\{\varepsilon_i\}$ and $\{e_i\}$. Other approaches that use only the energy eigenvalues, only the vacuum state, or only the effective potential, which is a small part of the scattering matrix (as represented by the effective action), do not use enough information, and thus are found lacking.

In this chapter I develop my approach to interpreting finite-volume, lattice theories as approximations to infinite-volume, continuum theories. In Section 3.1 I review Green's functions and show how they can be calculated. In Section 3.2 I

discuss renormalization and define physical coupling constants, which specify what theory we are approximating. In Section 3.3 I discuss qualitatively the sources of error in our calculation of physically significant quantities. Finally, in Section 3.4 I summarize what I have done and discuss prospects for future research.

3.1 Green's Functions

In this section I review complete and connected Green's functions, relate them to bound state energies and scattering amplitudes, and express Green's functions in terms of energy eigenvalues and eigenstates. The key results are Equations (3.10), (3.11), (3.15) and (3.23). Note that for simplicity I use infinite-volume, continuum notation, switching only at the end to finite-volume, lattice notation.

3.1.1 Review of Green's Functions, Bound State Energies and Scattering Amplitudes

Recall that *(complete) Green's functions* are defined as vacuum expectation values of time-ordered products:

$$G^{(k)}(x_1,\ldots,x_k) = \langle 0|\mathrm{T}\,\phi(x_1)\cdots\phi(x_k)|0\rangle. \tag{3.2}$$

Here the $x_i = (\mathbf{x}_i, t_i)$ are spacetime d-vectors. As usual, the time-ordering symbol T specifies that operators act from right to left in order of increasing time.

The Fourier transform of $G^{(k)}(x_1,\ldots,x_k)$ is

$$G^{(k)}(p_1,\ldots,p_k) = \int d^dx_1\cdots d^dx_k\, e^{i(p_1\cdot x_1+\cdots+p_k\cdot x_k)}\, G^{(k)}(x_1,\ldots,x_k), \tag{3.3}$$

where the $p_i = (\mathbf{p}_i, E_i)$ are momentum-energy d-vectors. Since the vacuum is translationally invariant, $G^{(k)}(p_1,\ldots,p_k)$ contains a total energy-momentum conservation delta function. Thus it is convenient to let

$$G^{(k)}(p_1,\ldots,p_k) = (2\pi)^d\delta^d(p_1+\cdots+p_k)\tilde{G}^{(k)}(p_1,\ldots,p_k), \tag{3.4}$$

where $\tilde{G}^{(k)}(p_1,\ldots,p_k)$ is only defined when $p_1+\cdots+p_k = 0$.

More interesting are *connected Green's functions*, defined recursively by the relation,

$$G^{(k)}(x_1,\ldots,x_k) = \sum_{\cup\mathcal{I}=K}\prod_{I\in\mathcal{I}} G_c^{|I|}(x_I), \tag{3.5}$$

where $K = \{1,\ldots,k\}$, $\mathcal{I}$ is a partition of K, and $x_I = \{x_{I(1)},\ldots,x_{I(|I|)}\}$, together with the initial condition $G^{(1)}(x_1) = G_c^{(1)}(x_1)$. In other words, $G^{(k)}(x_1,\ldots,x_k)$ is the sum over all partitions of $\{1,\ldots,k\}$ of products of connected Green's functions of subsets of $\{x_1,\ldots,x_k\}$. For example,

$$G^{(2)}(x_1,x_2) = G_c^{(2)}(x_1,x_2) + G_c^{(1)}(x_1)G_c^{(1)}(x_2), \tag{3.6a}$$

$$\begin{aligned} G^{(3)}(x_1,x_2,x_3) = {} & G_c^{(3)}(x_1,x_2,x_3) + G_c^{(1)}(x_1)G_c^{(2)}(x_2,x_3) + G_c^{(1)}(x_2)G_c^{(2)}(x_1,x_3) \\ & + G_c^{(1)}(x_3)G_c^{(2)}(x_1,x_2) + G_c^{(1)}(x_1)G_c^{(1)}(x_2)G_c^{(1)}(x_3). \end{aligned} \tag{3.6b}$$

We can also express connected Green's functions explicitly in terms of complete Green's functions:[1]

$$G_c^{(k)}(x_1,\ldots,x_k) = \sum_{\cup\mathcal{I}=K}(-1)^{|\mathcal{I}|-1}(|\mathcal{I}|-1)!\prod_{I\in\mathcal{I}} G^{|I|}(x_I). \tag{3.7}$$

For example,

$$\begin{aligned} G_c^{(3)}(x_1,x_2,x_3) = {} & G^{(3)}(x_1,x_2,x_3) - G^{(1)}(x_1)G^{(2)}(x_2,x_3) - G^{(1)}(x_2)G^{(2)}(x_1,x_3) \\ & - G^{(1)}(x_3)G^{(2)}(x_1,x_2) + 2\,G^{(1)}(x_1)G^{(1)}(x_2)G^{(1)}(x_3). \end{aligned} \tag{3.8}$$

We define $G_c^{(k)}(p_1,\ldots,p_k) = (2\pi)^d\delta^d(p_1+\cdots+p_k)\tilde{G}_c^{(k)}(p_1,\ldots,p_k)$. The virtue of connected Green's functions is that $\tilde{G}_c^{(k)}(p_1,\ldots,p_k)$ contains no total or partial energy-momentum conservation delta function. Thus $G_c^{(k)}(p_1,\ldots,p_k)$ contains only the exhibited delta function $(2\pi)^d\delta^d(p_1+\cdots+p_k)$. In contrast, complete Green's functions contain partial energy-momentum conservation delta functions through their

[1] This relation is most easily derived using the generating functional $G_c[J] = \ln G[J]$ of connected Green's functions, where $G[J]$ is the generating functional of complete Green's functions:

$$G_c^{(k)}(x_1,\ldots,x_k) = \frac{\delta}{\delta J(x_1)}\cdots\frac{\delta}{\delta J(x_k)}\ln G[J]\big|_{J=0}.$$

disconnected components. For example,

$$G^{(2)}(p_1,p_2) = G_c^{(2)}(p_1,p_2) + G_c^{(1)}(p_1)G_c^{(1)}(p_2) \tag{3.9a}$$

$$= (2\pi)^d\delta^d(p_1+p_2)\tilde{G}_c^{(2)}(p_1,p_2) + (2\pi)^d\delta^d(p_1)\tilde{G}_c^{(1)}(p_1)\,(2\pi)^d\delta^d(p_2)\tilde{G}_c^{(1)}(p_2). \tag{3.9b}$$

Note that $G_c^{(k)}(p_1,\ldots,p_k) = G^{(k)}(p_1,\ldots,p_k)$ unless the set $\{p_1,\ldots,p_k\}$ is *separable*, that is unless some nontrivial subset sums to zero.

The two-point Green's function is simply related to bound state energies. In particular, in an infinite-volume, continuum theory $\tilde{G}_c^{(2)}(p,-p)$ is a Lorentz invariant function of p, and thus can be viewed as a function of $p^2 = E^2 - |\mathbf{p}|^2$. Then $\tilde{G}_c^{(2)}(p^2)$ has a simple pole at $p^2 = m^2$ with residue iZ for each bound state with mass m:

$$\tilde{G}_c^{(2)}(p^2)|_{p^2=m^2} = \frac{iZ}{p^2-m^2}. \tag{3.10}$$

Here Z is a normalization constant. Since $\tilde{G}_c^{(2)}(p^2)$ is essentially an expectation value of products of fields, we can vary Z by rescaling the field ϕ, that is by varying λ_ϕ.

We could also try to determine bound state energies by simply looking at the energy eigenvalues. But it is not clear how to distinguish a bound state from other states. For example, consider the $\mathbf{p} = 0$ sector of an infinite-volume, continuum free theory. The lowest energy state is the vacuum, whose energy is conventionally set to zero. The next lowest energy state is the 1-particle rest state with energy m. It is the only bound state in the sector. The next lowest energy state consists of 2 particles at rest and has energy $2m$. Beyond this the spectrum is continuous. There are states with any energy $\geq 2m$, consisting of 2 particles with equal and opposite momenta. There is also a state with energy $3m$ consisting of 3 particles at rest, and then another continuous spectrum of energies $\geq 3m$. And so on. In a corresponding finite-volume, lattice theory the entire spectrum is discrete. Thus it is difficult to distinguish true bound states from states that are merely collections of bound states in motion with respect to each other.

Green's functions are simply related to scattering amplitudes. In particular, $G^{(k)}(p_1,\ldots,p_k)$ has a simple pole when any p_i is on-shell, that is at $p_i^2 = E_i^2 - |\mathbf{p}_i|^2 = m^2$ for each i, where m is the mass of a bound state. Up to a normalization constant,

the scattering amplitude S_{fi} for k incoming particles with energy-momentum p_i or outgoing particles with energy-momentum $-p_i$ is the residue of this multiple pole:

$$S_{fi} = (-iZ^{-1/2})^k\,(p_1^2-m^2)\cdots(p_k^2-m^2)\,G^{(k)}(p_1,\ldots,p_k). \tag{3.11}$$

If $\{p_1,\ldots,p_k\}$ is separable, then this amplitude includes processes in which a nontrivial subset of the k incoming or outgoing particles scatter amongst themselves without interacting with the remaining particles. Such processes are excluded from the amplitude if we use a connected Green's function instead of a complete Green's function.

Note that it is desirable that $G^{(1)}(x) = G_c^{(1)}(x) = \langle 0|\phi(x)|0\rangle$ is zero. Otherwise, we have nonzero scattering amplitudes for processes in which nonphysical particles with zero energy and zero momentum appear out of nothing or disappear into nothing. We can always arrange that $\langle 0|\phi(x)|0\rangle = 0$ by redefining the field $\phi \to \phi - \langle\phi\rangle$, which is equivalent to redefining the coupling constants λ_k upon expanding the lagrangian density. Doing so changes all of the complete Green's functions but has no effect on any connected Green's function, except for $G_c^{(1)}(x) = G^{(1)}(x)$.

One can relate connected Green's functions $G_c^{(k)}(p_1,\ldots,p_k)$ to vertex functions $\Gamma^{(k)}(x_1,\ldots,x_k)$, which are the fundamental objects in perturbation theory, renormalization and the study of spontaneous symmetry breaking. But I do not use vertex functions, because complete and connected Green's functions are more directly calculated in the hamiltonian formalism.

In summary, if we can calculate Green's functions, then we can determine the physical states of the theory—the bound states—and the scattering amplitudes between collections of these states.

3.1.2 Calculation of Complete Green's Functions

I want to relate Green's functions to energy eigenvalues and energy eigenstates. The problem is that we consider a fixed time in the hamiltonian formalism, whereas Green's functions are defined as vacuum expectation values of time-ordered products of operators at various times. The solution is to translate everything to a single fixed time.

In particular, from the definition (3.2) of $G^{(k)}(x_1,\ldots,x_k)$ and of its Fourier transform (3.3),

$$G^{(k)}(p_1,\ldots,p_k) = \sum_{\rho\in S_k}\int d^dx_1\cdots d^dx_k\,\theta(t_1,\ldots,t_k)\,e^{i(p_{\rho(1)}\cdot x_1+\cdots+p_{\rho(k)}\cdot x_k)}\,\langle 0|\phi(x_1)\cdots\phi(x_k)|0\rangle, \quad (3.12)$$

where ρ is a permutation of $\{1,\ldots,k\}$, and $\theta(t_1,\ldots,t_k)=\theta(t_1-t_2)\cdots\theta(t_{k-1}-t_k)$ is 1 if $t_1\geq\cdots\geq t_k$ and 0 otherwise.

Inserting a complete set $\{\alpha\}$ of energy eigenstates between each pair of $\phi(x_i)$ and using the definition, $\phi(x)=e^{iHt}\phi(\mathbf{x})e^{-iHt}$,

$$\begin{aligned}G^{(k)}(p_1,\ldots,p_k) &= \sum_{\rho\in S_k}\int d^dx_1\cdots d^dx_k\,\theta(t_1,\ldots,t_k)\,e^{i(p_{\rho(1)}\cdot x_1+\cdots+p_{\rho(k)}\cdot x_k)}\\ &\quad\times\langle 0|e^{iHt_1}\phi(\mathbf{x}_1)e^{-iHt_1}\sum_{\alpha_1}|\alpha_1\rangle\langle\alpha_1|\cdots\\ &\quad\times e^{iHt_{k-1}}\phi(\mathbf{x}_{k-1})e^{-iHt_{k-1}}\sum_{\alpha_{k-1}}|\alpha_{k-1}\rangle\langle\alpha_{k-1}|e^{iHt_k}\phi(\mathbf{x}_k)e^{-iHt_k}|0\rangle. \quad (3.13)\end{aligned}$$

Now each $e^{\pm iHt}$ becomes $e^{\pm i\varepsilon_\alpha t}$, where ε_α is the energy of some eigenstate α. We can perform the spatial integrals using the definition (2.11) of $\tilde\phi(\mathbf{p})$, and the temporal integrals by parts. Each $\theta(t_i-t_{i+1})$ becomes $\delta(t_i-t_{i+1})$ and the t_i integral can be eliminated. Thus

$$\begin{aligned}G^{(k)}(p_1,\ldots,p_k) &= 2\pi\delta(E_1+\cdots+E_k)\sum_{\rho\in S_k}\langle 0|\tilde\phi(\mathbf{p}_{\rho(1)})\sum_{\alpha_1}\frac{i}{E_{\rho(1)}-\Delta\varepsilon_{\alpha_1}}|\alpha_1\rangle\langle\alpha_1|\cdots\\ &\quad\times\tilde\phi(\mathbf{p}_{\rho(k-1)})\sum_{\alpha_{k-1}}\frac{i}{E_{\rho(1)}+\cdots+E_{\rho(k-1)}-\Delta\varepsilon_{\alpha_{k-1}}}|\alpha_{k-1}\rangle\langle\alpha_{k-1}|\tilde\phi(\mathbf{p}_{\rho(k)})|0\rangle, \quad (3.14)\end{aligned}$$

where $\Delta\varepsilon_\alpha=\varepsilon_\alpha-\varepsilon_0$ is the energy of the state α relative to the vacuum. Here I assume the exponentials vanish at $t=\pm\infty$.[2]

Finally, $G^{(k)}(p_1,\ldots,p_k)$ contains the factor $(2\pi)^d\delta^d(p_1+\cdots+p_k)$ (infinite-volume) or $2\pi\delta(E_1+\cdots+E_k)L^{d-1}\delta_{\mathbf{p}_1+\cdots+\mathbf{p}_k}$ (finite-volume). In order to approximate

[2]For example, we could ensure the convergence of the t-integrals by substituting $\varepsilon_0+i\delta$ for ε_0 in the initial and final vacuum states, thus suppressing terms as $t_1\to+\infty$ or $t_k\to-\infty$, and then taking the limit $\delta\to 0$.

the infinite-volume theory by a finite-volume theory, I focus on $\tilde G^{(k)}(p_1,\ldots,p_k)$. In a finite-volume theory

$$\begin{aligned}\tilde G^{(k)}(p_1,\ldots,p_k) &= L^{-(d-1)}\sum_{\rho\in S_k}\langle 0|\tilde\phi_{\mathbf{p}_{\rho(1)}}\sum_{\alpha_1}\frac{i}{E_{\rho(1)}-\Delta\varepsilon_{\alpha_1}}|\alpha_1\rangle\langle\alpha_1|\cdots\\ &\quad\times\tilde\phi_{\mathbf{p}_{\rho(k-1)}}\sum_{\alpha_{k-1}}\frac{i}{E_{\rho(1)}+\cdots+E_{\rho(k-1)}-\Delta\varepsilon_{\alpha_{k-1}}}|\alpha_{k-1}\rangle\langle\alpha_{k-1}|\tilde\phi_{\mathbf{p}_{\rho(k)}}|0\rangle, \quad (3.15)\end{aligned}$$

This last expression is the desired result and is a generalization of the Källen-Lehmann representation of $G^{(2)}(x_1,x_2)$. I have eliminated all explicit references to time: The matrix element can be evaluated using the energy eigenstates of the hamiltonian formalism, which are defined for some fixed but arbitrary time. Thus we can calculate complete Green's functions using energy eigenvalues, energy eigenstates and $\tilde\phi_{\mathbf{p}}$ matrix elements between energy eigenstates.

In practice, we use the energy eigenstate basis. Then the vacuum $|0\rangle$ is a column vector, $\tilde\phi_{\mathbf{p}}$ is a matrix which connects states that differ in total momentum by $\mathbf{p}$ and in parity, and $\sum_\alpha\frac{i}{E-\Delta\varepsilon_\alpha}|\alpha\rangle\langle\alpha|$ is a diagonal matrix. We calculate $\tilde G^{(k)}(p_1,\ldots,p_k)$ by starting with the column vector $|0\rangle$, successively multiplying by matrices, and then multiplying by the row vector $\langle 0|$. Each matrix multiplication is an $O(n^2)$ or an $O(n)$ operation, and the final multiplication by $\langle 0|$ is an $O(1)$ operation. Thus the entire calculation requires no more than $O(n^2)$ time.

Then we sum over all permutations ρ. If not all p_i are distinct, then the number of inequivalent permutations is reduced. In particular, if $p_1=\cdots=p_k=0$, then all permutations are equivalent and we need only multiply by $k!$.

But we have a problem. If the set $\{p_1,\ldots,p_k\}$ is separable, that is if some nontrivial subset sums to zero, then the expression (3.15) for $\tilde G^{(k)}(p_1,\ldots,p_k)$ is ill-defined. In particular, the factor $\frac{i}{E-\Delta\varepsilon_\alpha}$ is divergent for ρ such that $E=E_{\rho(1)}+\cdots+E_{\rho(j)}=0$ and $\alpha=0$, that is $\Delta\varepsilon_\alpha=0$. In fact, a more careful analysis using the $i\delta$ convergence term shows that such factors are related to the partial energy-momentum conservation delta functions in the disconnected components of $\tilde G^{(k)}(p_1,\ldots,p_k)$. Nevertheless, the expression for $\tilde G^{(k)}(p_1,\ldots,p_k)$ is unsuitable for numerical calculations when the set $\{p_1,\ldots,p_k\}$ is separable.

We could simply avoid sets $\{p_1, \ldots, p_k\}$ that are separable. But we have a problem even if the set $\{p_1, \ldots, p_k\}$ is almost separable, that is if some nontrivial subset sums to almost zero. In this case, the troublesome factors $\frac{i}{E-\Delta\epsilon_\alpha}$ are not divergent but merely very large. Then certain combinations of terms, some including these large factors, sum to exactly zero and correspond to disconnected components of $\tilde{G}^{(k)}(p_1, \ldots, p_k)$. Thus we lose a lot of accuracy when we numerically calculate $\tilde{G}^{(k)}(p_1, \ldots, p_k)$.

We could calculate connected Green's functions instead of complete Green's functions, as I show how to do in the next subsection, since the divergences are related to the disconnected components of $\tilde{G}^{(k)}(p_1, \ldots, p_k)$. Unfortunately, doing so increases the computation time, perhaps to an unacceptable degree. Alternatively, we could simply use high-precision arithmetic, which may give us acceptable accuracy, especially if there are other sources of large error.

3.1.3 Calculation of Connected Green's Functions

In order to avoid the divergences associated with disconnected components of complete Green's functions, I want to directly calculate connected Green's functions. First, consider $G_c^{(k)}(x_1, \ldots, x_k)$, where $t_1 \geq \cdots \geq t_k$. Then from the defining relation (3.7),

$$G_c^{(k)}(x_1, \ldots, x_k) = \sum_{\cup \mathcal{I}=K} (-1)^{|\mathcal{I}|-1}(|\mathcal{I}|-1)! \prod_{I \in \mathcal{I}} \langle 0|\phi(x_{I(1)}) \cdots \phi(x_{I(|I|)})|0\rangle, \tag{3.16}$$

where we can drop the time-ordering symbol so long as each $I \in \mathcal{I}$ is ordered: $I(1) < \cdots < I(|I|)$.

Now we can insert $1_\nu = |0\rangle\langle 0| + Q$ between each pair of $\phi(x_i)$, where $Q = \sum_{\alpha \neq 0} |\alpha\rangle\langle\alpha|$. I treat the vacuum state differently, since its appearance is related to the divergences in complete Green's functions. Then we can simplify the expression above by combining terms. For example,

$$G_c^{(2)}(x_1, x_2) = \langle 0|\phi(x_1)\phi(x_2)|0\rangle - \langle 0|\phi(x_1)|0\rangle\langle 0|\phi(x_2)|0\rangle = \langle 0|\phi(x_1)Q\phi(x_2)|0\rangle. \tag{3.17a}$$

Similarly,

$$G_c^{(3)}(x_1, x_2, x_3) = \langle 0|\phi(x_1)Q\phi(x_2)Q\phi(x_3)|0\rangle - \langle 0|\phi(x_2)|0\rangle\langle 0|\phi(x_1)Q\phi(x_3)|0\rangle \tag{3.17b}$$

and

$$\begin{aligned} G_c^{(4)}(x_1, x_2, x_3, x_4) &= \langle 0|\phi(x_1)Q\phi(x_2)Q\phi(x_3)Q\phi(x_4)|0\rangle \\ &- \langle 0|\phi(x_2)|0\rangle\langle 0|\phi(x_1)Q\phi(x_3)Q\phi(x_4)|0\rangle - \langle 0|\phi(x_3)|0\rangle\langle 0|\phi(x_1)Q\phi(x_2)Q\phi(x_4)|0\rangle \\ &- \langle 0|\phi(x_1)Q\phi(x_3)|0\rangle\langle 0|\phi(x_2)Q\phi(x_4)|0\rangle - \langle 0|\phi(x_1)Q\phi(x_4)|0\rangle\langle 0|\phi(x_2)Q\phi(x_3)|0\rangle \\ &+ \langle 0|\phi(x_2)|0\rangle\langle 0|\phi(x_3)|0\rangle\langle 0|\phi(x_1)Q\phi(x_4)|0\rangle. \end{aligned} \tag{3.17c}$$

The corresponding expressions for $G_c^{(5)}$, $G_c^{(6)}$, $G_c^{(7)}$ and $G_c^{(8)}$ have 22, 92, 426 and 2146 nonzero terms, respectively.

In general, one finds that

$$G_c^{(k)}(x_1, \ldots, x_k) = \sum_{\cup \mathcal{I}=K} g(\mathcal{I}) \prod_{I \in \mathcal{I}} \langle 0|\phi(x_{I(1)})Q \cdots \phi(x_{I(|I|-1)})Q\phi(x_{I(|I|)})|0\rangle, \tag{3.18}$$

where $g(\mathcal{I})$ is an integer, which can be directly, if tediously, calculated.

If $G^{(1)}(x) = \langle 0|\phi(x)|0\rangle = 0$, then the number of nonzero terms in the expression for $G_c^{(k)}(x_1, \ldots, x_k)$ is reduced, since the term for any partition containing a singleton set is zero. In particular, if $\langle 0|\phi(x)|0\rangle = 0$, the expressions for $G_c^{(3)}, \ldots, G_c^{(8)}$ have only 1, 3, 9, 33, 135 and 609 nonzero terms, respectively.

If the potential density $V(\phi)$ is even in ϕ, then the vacuum has even parity. In this case, the number of nonzero terms in the expression for $G_c^{(k)}(x_1, \ldots, x_k)$ is further reduced, since the vacuum expectation value of an odd number of $\phi(x_i)$ is zero. In particular, if the potential density $V(\phi)$ is even in ϕ, the expressions for $G_c^{(4)}$, $G_c^{(6)}$ and $G_c^{(8)}$ have only 3, 24 and 312 nonzero terms, respectively.

Let $s^+(i, \mathcal{I})$ be the successor of i in the ordered partition $\mathcal{I}$ and $s^-(i, \mathcal{I})$ be the predecessor. For example, if $\mathcal{I} = \{(1,3),(2,4)\}$, corresponding to the fourth term in the expression (3.17c) for $G_c^{(4)}(x_1, x_2, x_3, x_4)$, then $s^+(1, \mathcal{I}) = 3$, $s^-(3, \mathcal{I}) = 1$ and $s^-(1, \mathcal{I}) = s^+(3, \mathcal{I}) = 0$. Note that the predecessor of 1 and the successor of k are always 0, since each set in the partition is ordered.

Then expanding each Q,

$$G_c^{(k)}(x_1, \ldots, x_k) = \sum_{\cup \mathcal{I}=K} g(\mathcal{I}) \sum_{\substack{\alpha_1, \ldots, \alpha_k \\ \beta_1, \ldots, \beta_k}}^{*} \prod_{i=1}^{k} \langle \beta_i|\phi(x_i)|\alpha_i\rangle, \tag{3.19}$$

where in the starred sum

$$\alpha_i = \begin{cases} 0, & \text{if } s^+(i,\mathcal{I}) = 0; \\ \beta_{s^+(i,\mathcal{I})} \neq 0, & \text{otherwise,} \end{cases} \tag{3.20a}$$

$$\beta_i = \begin{cases} 0, & \text{if } s^-(i,\mathcal{I}) = 0; \\ \alpha_{s^-(i,\mathcal{I})} \neq 0, & \text{otherwise.} \end{cases} \tag{3.20b}$$

Continuing my example,

$$\begin{aligned} &G_c^{(4)}(x_1,x_2,x_3,x_4) \\ &\quad = -\langle 0|\phi(x_1)Q\phi(x_3)|0\rangle\langle 0|\phi(x_2)Q\phi(x_4)|0\rangle + 5 \text{ other terms} \qquad (3.21a) \\ &\quad = -\sum_{\substack{\alpha_1,\ldots,\alpha_4 \\ \beta_1,\ldots,\beta_4}}^{*} \langle\beta_1|\phi(x_1)|\alpha_1\rangle\langle\beta_3|\phi(x_3)|\alpha_3\rangle\langle\beta_2|\phi(x_2)|\alpha_2\rangle\langle\beta_4|\phi(x_4)|\alpha_4\rangle \\ &\qquad + 5 \text{ other terms,} \qquad (3.21b) \end{aligned}$$

where $\beta_1 = 0$, $\alpha_1 = \beta_3 \neq 0$, $\alpha_3 = \beta_2 = 0$, $\alpha_2 = \beta_4 \neq 0$, and $\alpha_4 = 0$. Thus the sum is effectively over $\alpha_1, \alpha_2 \neq 0$.

Consider $G_c^{(k)}(p_1,\ldots,p_k)$. The following derivation parallels that for complete Green's functions in the previous subsection. Using the expression (3.19) for $G_c^{(k)}(x_1,\ldots,x_k)$ and the definition of $G_c^{(k)}(p_1,\ldots,p_k)$ as a Fourier transform of $G_c^{(k)}(x_1,\ldots,x_k)$,

$$\begin{aligned} G_c^{(k)}(p_1,\ldots,p_k) = \sum_{\rho\in S_k} \int d^dx_1\cdots d^dx_k\, \theta(t_1,\ldots,t_k)\, e^{i(p_{\rho(1)}\cdot x_1+\cdots+p_{\rho(k)}\cdot x_k)} \\ \times \sum_{\cup\mathcal{I}=K} g(\mathcal{I}) \sum_{\substack{\alpha_1,\ldots,\alpha_k \\ \beta_1,\ldots,\beta_k}}^{*} \prod_{i=1}^{k} \langle\beta_i|\phi(x_i)|\alpha_i\rangle. \end{aligned} \tag{3.22}$$

Using the definition, $\phi(x) = e^{iHt}\phi(\mathbf{x})e^{-iHt}$, performing the spatial and temporal integrals, and factoring out the total energy-momentum conservation delta function for a finite-volume theory,

$$\begin{aligned} &\tilde{G}_c^{(k)}(p_1,\ldots,p_k) \\ &\quad = L^{-(d-1)} \sum_{\rho\in S_k} \sum_{\cup\mathcal{I}=K} g(\mathcal{I}) \sum_{\substack{\alpha_1,\ldots,\alpha_k \\ \beta_1,\ldots,\beta_k}}^{*} \left[\prod_{i=1}^{k} \langle\beta_i|\tilde{\phi}_{\mathbf{p}_{\rho(i)}}|\alpha_i\rangle\right] \frac{i}{E_{\rho(1)} - (\varepsilon_{\alpha_1} - \varepsilon_{\beta_1})} \cdots \\ &\qquad \times \frac{i}{E_{\rho(1)}+\cdots+E_{\rho(k-1)} - (\varepsilon_{\alpha_1}+\cdots+\varepsilon_{\alpha_{k-1}} - \varepsilon_{\beta_1} - \cdots - \varepsilon_{\beta_{k-1}})}. \end{aligned} \tag{3.23}$$

This is the desired result.

Continuing my example,

$$\begin{aligned} &\tilde{G}_c^{(4)}(p_1,p_2,p_3,p_4) \\ &\quad = L^{-(d-1)} \sum_{\rho\in S_k} \Big\{ \\ &\qquad - \sum_{\alpha_1,\alpha_2\neq 0} \langle 0|\tilde{\phi}_{\mathbf{p}_{\rho(1)}}|\alpha_1\rangle\langle\alpha_1|\tilde{\phi}_{\mathbf{p}_{\rho(3)}}|0\rangle\langle 0|\tilde{\phi}_{\mathbf{p}_{\rho(2)}}|\alpha_2\rangle\langle\alpha_2|\tilde{\phi}_{\mathbf{p}_{\rho(4)}}|0\rangle \\ &\qquad \frac{i}{E_{\rho(1)} - \Delta\varepsilon_{\alpha_1}} \frac{i}{E_{\rho(1)} + E_{\rho(2)} - \Delta\varepsilon_{\alpha_1} - \Delta\varepsilon_{\alpha_2}} \frac{i}{E_{\rho(1)} + E_{\rho(2)} + E_{\rho(3)} - \Delta\varepsilon_{\alpha_2}} \\ &\qquad + 5 \text{ other terms} \Big\}. \end{aligned} \tag{3.24}$$

In a free theory, there are k-particle energy eigenstates $|\mathbf{p}_1,\ldots,\mathbf{p}_k\rangle$ with energies $\omega_{\mathbf{p}_1} + \cdots + \omega_{\mathbf{p}_k}$. The operator $\tilde{\phi}_{\mathbf{p}}$ destroys a particle with momentum $\mathbf{p}$ or creates a particle with momentum $-\mathbf{p}$. It is straightforward, if tedious, to verify that expression (3.23) specialized to $\tilde{G}_c^{(4)}(p_1,p_2,p_3,p_4)$ is zero, as expected.

In general, one finds that the $\varepsilon = \varepsilon_{\alpha_1} + \cdots + \varepsilon_{\alpha_j} - \varepsilon_{\beta_1} - \cdots - \varepsilon_{\beta_j}$ terms are nonzero for all $\mathcal{I}$ such that $g(\mathcal{I}) \neq 0$ (assuming the theory is massive). Thus we have, in fact, eliminated the divergences related to the disconnected components of $\tilde{G}^{(k)}(p_1,\ldots,p_k)$.

Unfortunately, some $\frac{i}{E-\varepsilon}$ factors now depend on more than one α_i, so the sums over states cannot be performed sequentially, as they can for complete Green's functions. Thus the time to compute a connected Green's function is greater than the time to compute the corresponding complete Green's function. In particular, a careful analysis shows that the time to compute $\tilde{G}_c^{(k)}(p_1,\ldots,p_k)$ is $O(n^{\lfloor k/2\rfloor})$. Thus the time to compute high-order connected Green's functions is prohibitive.

In summary, we can compute the complete Green's functions for a nonseparable set $\{p_1,\ldots,p_k\}$ using Equation (3.15), in which case the complete and connected Green's functions are equal. The connected Green's function for a separable set can be approximated by substituting an approximately equal nonseparable set. The computation time is no more than $O(n^2)$, but the accuracy is low for almost separable sets, unless we use high-precision arithmetic. Alternatively, we can directly compute the connected Green's function for any set $\{p_1,\ldots,p_k\}$ using Equation (3.23). The accuracy is high, but the computation time is $O(n^{\lfloor k/2\rfloor})$.

3.2 Renormalization

3.2.1 General Renormalization Scheme

We want to approximate some infinite-volume, continuum theory by a finite-volume, lattice theory. A finite-volume, lattice ϕ^r theory is specified by assigning values to the $r+2$ quantities $\lambda_\phi, \lambda_0, \ldots, \lambda_r$, collectively denoted by λ, setting $\lambda_k = 0$ for $k > r$, and assigning values to L and a. We want the finite-volume, lattice theory to approach a limit, the infinite-volume, continuum theory, as $L \to \infty$ and $a \to 0$. In general, the limit does not exist if we fix λ as we take limits: The theory diverges.

But we can obtain a well-defined limit theory if we carefully vary, that is renormalize, λ as $L \to \infty$ and $a \to 0$. Note that in my approach renormalization is not necessary to eliminate infinities: Any model specified by λ, L and a is a well-defined, finite quantum mechanical model. But renormalization is necessary in order to fix what theory is being approximated! Indeed, the coupling constants λ are not physical coupling constants but bare coupling constants. They have no physical significance independent of L and a, but merely serve to parameterize a class of models for each choice of L and a. Thus it is not physically meaningful to fix λ as $L \to \infty$ and $a \to 0$.

In order to obtain a well-defined limit theory, we need to fix $r+2$ quantities, collectively denoted by λ^{phys}, that have physical significance independent of L and a. In a model specified by λ, L and a these physical coupling constants have particular values:

$$\lambda^{\text{phys}} = \lambda^{\text{phys}}(\lambda; L, a). \tag{3.25}$$

In principle, this relation can be inverted:

$$\lambda = \lambda(\lambda^{\text{phys}}; L, a). \tag{3.26}$$

The connected Green's function $\tilde{G}_c^{(k)}(p_1, \ldots, p_k)$ depends on λ, L and a, as well as $p_1, \ldots, p_k$. Thus $\tilde{G}_c^{(k)}(p_1, \ldots, p_k)$ depends on λ^{phys}, L and a, since λ implicitly depends on λ^{phys}, L and a:

$$\tilde{G}_c^{(k)}(p_1, \ldots, p_k) = \tilde{G}_c^{(k)}(p_1, \ldots, p_k; \lambda^{\text{phys}}; L, a). \tag{3.27}$$

Then we can define $\tilde{G}_c^{(k)}(p_1, \ldots, p_k)$ in the infinite-volume and continuum limits while

fixing λ^{phys}:

$$\tilde{G}_c^{(k)}(p_1, \ldots, p_k; \lambda^{\text{phys}}) = \lim_{\substack{L \to \infty \\ a \to 0}} \tilde{G}_c^{(k)}(p_1, \ldots, p_k; \lambda^{\text{phys}}; L, a). \tag{3.28}$$

Mathematical subtleties aside, this equation defines quantum field theory in the infinite-volume and continuum limits. Physicists generally believe that the limits exist—at least for renormalizable theories—although this has been proven in only a few special cases.

We want to approximate $\tilde{G}_c^{(k)}(p_1, \ldots, p_k; \lambda^{\text{phys}})$ by $\tilde{G}_c^{(k)}(p_1, \ldots, p_k; \lambda^{\text{phys}}; L, a)$. We expect to get a sufficiently good approximation by taking L sufficiently large and a sufficiently small, as is required by the existence of the limit. In practice, we specify λ^{phys}. Then we choose L and a. Then we can solve for λ to any desired degree of accuracy by inverting the relation between λ^{phys} and λ, using any standard numerical iteration method. Thus we must compute λ^{phys} for several choices of λ until we find the approximately correct values of λ. We may be able to accelerate the iteration process by calculating $\partial\lambda^{\text{phys}}/\partial\lambda$. Finally, we can calculate interesting Green's functions, and hence bound state energies and scattering amplitudes.

3.2.2 Specific Choice of Renormalization Conditions

In order to apply the general concepts of the previous subsection, we need to choose quantities λ^{phys} to serve as physical coupling constants. To a certain extent the choice is arbitrary and can be made for convenience. It is generally believed that all reasonable renormalization conditions lead to the same class of limit theories. The usual approach is to choose vertex functions $\Gamma^{(k)}(p_1, \ldots, p_k)$ at particular points to be physical coupling constants. But in the hamiltonian formalism connected Green's functions are more easily calculated.

In particular, I choose $\lambda_\phi^{\text{phys}} = Z$, $\lambda_0^{\text{phys}} = \varepsilon_0/L^{d-1}$ (the energy density of the vacuum) and $\lambda_k^{\text{phys}} = \tilde{G}_c^{(k)}(0, \ldots, 0)$, for $k = 1, \ldots, r$, to be physical coupling constants. Note that we must choose each $\mathbf{p}_i = 0$ in $\tilde{G}_c^{(k)}$, since this is the only momentum common to all lattices. In contrast, each E_i is continuous and can be chosen arbitrarily. I choose each $E_i = 0$ for simplicity and symmetry.

We can calculate $\lambda_k^{\text{phys}} = \tilde{G}_c^{(k)}(0, \ldots, 0)$, for $k = 1, \ldots, r$, directly using

Equation (3.23). Since all p_i are equal, the sum over permutations ρ can be replaced by multiplication by $k!$. Alternatively, we can approximate λ_k^{phys} by $\tilde{G}^{(k)}(p_1,\ldots,p_k)$ using Equation (3.15), where $\{p_1,\ldots,p_k\}$ is a nonseparable set close to $\{0,\ldots,0\}$.

In order to calculate $\lambda_\phi^{\text{phys}} = Z$, we need to calculate $\tilde{G}_c^{(2)}(p,-p)$. Specializing Equation (3.23) and using Equation (2.18) for $\tilde{\phi}_{\mathbf{p}}$,

$$\tilde{G}_c^{(2)}(p,-p) = \frac{1}{\omega_{\mathbf{p}}\lambda_\phi}\sum_{\alpha\neq 0}|\langle\alpha|(a_{\mathbf{p}}+a_{-\mathbf{p}}^\dagger)|0\rangle|^2\Delta\varepsilon_\alpha\frac{i}{E^2-(\Delta\varepsilon_\alpha)^2}, \tag{3.29}$$

where I have used the symmetry between eigenstates with momentum $\mathbf{p}$ and $-\mathbf{p}$.

In an infinite-volume, continuum theory $\tilde{G}_c^{(2)}(p,-p)$ is a Lorentz invariant function of p, but the introduction of a lattice breaks Lorentz invariance. Thus in a finite-volume, lattice theory I define iZ as the residue of the simple pole in $\tilde{G}_c^{(2)}(E^2,\mathbf{p}=0)$ at $E^2=m^2$. It is clear that this pole comes from the term where α is the 1-particle rest state $|1\rangle$, which is the lowest energy bound state. This state is the lowest energy eigenstate aside from the vacuum, has zero momentum, and has odd parity if the potential density $V(\phi)$ is even in ϕ. Thus the 1-particle rest state is easily identified. Then

$$\lambda_\phi^{\text{phys}} = Z = \frac{m}{\mu\lambda_\phi}|\langle 1|(a_0+a_0^\dagger)|0\rangle|^2, \tag{3.30}$$

which is easily calculated if $|0\rangle$ and $|1\rangle$ are known. Recall that $\mu=\omega_0$ is the mass of fictitious free particles. Note that $Z=\lambda_\phi^{-1}$ in a free theory.

Finally, there are $r+2$ degrees of freedom, represented by λ or λ^{phys}, in a ϕ^r model. But 2 of these degrees of freedom correspond to merely a linear redefinition of the field. Such a redefinition changes the Green's functions but not the scattering amplitudes, and hence is physically insignificant. Another degree of freedom corresponds to merely a shift in energy scale, which is physically insignificant since only energy differences are measurable. We can always shift the energy scale by changing λ_0. Thus it is desirable to require that

$$\lambda_\phi^{\text{phys}} = Z = 1, \tag{3.31a}$$

$$\lambda_0^{\text{phys}} = \frac{\varepsilon_0}{L^{d-1}} = 0, \tag{3.31b}$$

$$\lambda_1^{\text{phys}} = \langle 0|\phi|0\rangle = 0. \tag{3.31c}$$

The theory is specified by the $r-1$ physically significant parameters $\lambda_2^{\text{phys}},\ldots,\lambda_r^{\text{phys}}$.

Note that in a theory such that the potential density $V(\phi)$ is even in ϕ, $\langle 0|\phi|0\rangle = 0$. But if $V(\phi)$ does not have a global minimum at $\phi=0$, then we anticipate spontaneous symmetry breaking, that is $\langle 0|\phi|0\rangle \neq 0$. The difficulty is that spontaneous symmetry breaking does not occur in finite systems but only in infinite systems. In order to handle spontaneous symmetry breaking in a finite-volume, lattice theory, we must break the symmetry by hand. For example, we could replace $V(\phi)$ by $V(\phi)+\Lambda\phi$, where Λ is a small external field coupled to ϕ, and then let $\Lambda\to 0$. In this case, the order of limits is important: We must let $L\to\infty$ and $a\to 0$ before $\Lambda\to 0$, otherwise there would be no symmetry breaking.

In summary, we can calculate physical coupling constants by calculating Green's functions (and the vacuum energy), and thereby determine what theory we are approximating.

3.3 Sources of Error

We can approximate Green's functions $\tilde{G}_c^{(k)}(p_1,\ldots,p_k;\lambda^{\text{phys}})$ in an infinite-volume, continuum theory by Green's functions $\tilde{G}_c^{(k)}(p_1,\ldots,p_k;\lambda^{\text{phys}};L,a)$ in a corresponding finite-volume, lattice theory, which can be calculated as I have described. In this section I discuss sources of error in the calculation. My discussion is qualitative.

My starting point is Equation (3.15) or (3.23), which expresses complete or connected Green's functions, respectively, in terms of energy eigenvalues and eigenstates. First, we do not know the exact energy eigenvalues and eigenstates but only approximations to them. As I discussed in Section 1.2, we can estimate the eigenvalue and eigenstate errors. Furthermore, although I have not discussed in detail how, we could also estimate the errors in $\tilde{\phi}_{\mathbf{p}}$ matrix elements between energy eigenstates due to errors in the eigenstates. Then the errors in energy eigenvalues and $\tilde{\phi}_{\mathbf{p}}$ matrix elements lead to errors in Green's functions.

Second, Equation (3.15) or (3.23) for complete or connected Green's functions, respectively, involves sums over all energy eigenstates (with the proper momentum and parity). Of course, there is an infinite number of such eigenstates, but we can calculate and sum over only a finite number of these. Thus there are errors in

Green's functions due to our truncating the sums over eigenstates.

But note that the operator $\tilde{\phi}_{\mathbf{p}}$ destroys one fictitious free particle with momentum $\mathbf{p}$ or creates one fictitious free particle with momentum $-\mathbf{p}$, as can be seen from Equation (2.18). In a free theory the operator $\tilde{\phi}_{\mathbf{p}}$ connects a given energy eigenstate to no more than two other eigenstates. Thus in a free theory only a finite number of terms in the expression for a Green's function are nonzero. In a theory with weak coupling, we expect roughly the same situation, that is only a finite number of terms contribute significantly to a particular Green's function. In general, using the orthogonality of eigenstates, we could put limits on the errors in Green's functions due to our truncating the sums over eigenstates.

Third, Equation (3.15) or (3.23) for complete or connected Green's functions, respectively, depends on the bare coupling constants λ. But we are interested in Green's functions as functions of physical coupling constants λ^{phys}. Since the λ^{phys} are themselves related to Green's functions (or the vacuum energy ε_0), there are errors in calculating λ^{phys} in terms of λ, and hence in inverting the relation and calculating λ in terms of λ^{phys}. If we quantify the two types of errors discussed above, then errors in Green's functions associated with errors in the bare coupling constants can be quantified using $\partial G/\partial\lambda$.

Lastly and most importantly, any finite-volume lattice theory is merely an approximation to some infinite-volume, continuum theory. Even if we could calculate the correct bare coupling constants λ as functions of the physical coupling constants λ^{phys}, and then calculate the exact Green's functions $\tilde{G}_c^{(k)}(p_1,\ldots,p_k;\lambda^{\text{phys}};L,a)$, we would still have errors since we are working with a finite model of the infinite theory of interest. Unfortunately, these errors are difficult to control.

For example, we can see from Equation (3.29) that $\tilde{G}_c^{(2)}(p,-p;\lambda^{\text{phys}};L,a)$ has, in general, an infinite number of simple poles, one at $E^2=\varepsilon_\alpha^2$ for each energy eigenstate α with momentum $\mathbf{p}$. Unfortunately, in the infinite-volume, continuum theory $\tilde{G}_c^{(2)}(p,-p;\lambda^{\text{phys}})$ has only a few simple poles, one for each bound state. Thus the difference between $\tilde{G}_c^{(2)}(p,-p;\lambda^{\text{phys}};L,a)$ and $\tilde{G}_c^{(2)}(p,-p;\lambda^{\text{phys}})$ is infinite at an infinite number of points!

We can see this phenomenon another way. For a theory with weak coupling, perturbation theory (Feynman diagrams) works well. To the zero-loop level the

Feynman diagrams for a finite-volume, lattice theory and the corresponding infinite-volume, continuum theory are essentially the same. But to the one-loop or higher level the Feynman diagrams for an infinite-volume, continuum theory involve nontrivial integrals over one or more internal d-momenta:

$$\tilde{G}_c^{(k)}(p_1,\ldots,p_k;\lambda^{\text{phys}}) = \int\frac{d^dp_1}{(2\pi)^d}\cdots\frac{d^dp_j}{(2\pi)^d}\frac{i}{p_1^2-m^2}\cdots\frac{i}{p_j^2-m^2}\cdots. \tag{3.32}$$

In a finite-volume, lattice theory the spatial parts of these integrals are replaced by finite sums:

$$\tilde{G}_c^{(k)}(p_1,\ldots,p_k;\lambda^{\text{phys}};L,a) = L^{-j(d-1)}\sum_{\mathbf{p}_1,\ldots,\mathbf{p}_j}\int\frac{dE_1}{(2\pi)}\cdots\frac{dE_j}{(2\pi)}\frac{i}{p_1^2-m^2}\cdots\frac{i}{p_j^2-m^2}\cdots. \tag{3.33}$$

Simple power counting shows that all of the energy integrals are convergent. We can easily perform these integrals by closing the contours in the complex energy planes, using the standard prescription for the contours to go around poles, and calculating the residue for each pole inside a contour. In general, the result is a function of the external energies that has poles at locations that depend on the external and internal momenta. When we sum over internal momenta, the number of poles increases. When we sum over diagrams, the number of poles increases further.

In any case, $\tilde{G}_c^{(k)}(p_1,\ldots,p_k;\lambda^{\text{phys}};L,a)$ may converge to $\tilde{G}_c^{(k)}(p_1,\ldots,p_k;\lambda^{\text{phys}})$ as $L\to\infty$ and $a\to 0$, but the convergence is not uniform or even pointwise. The limit is not so well behaved.

I would like to understand the nature of the infinite-volume and continuum limits, and to put bounds on the difference between a finite-volume, lattice Green's function and the corresponding infinite-volume, continuum Green's function. Then my method would be essentially complete. I could program a computer to calculate finite-volume, lattice Green's functions and to quantify the errors. Then, in principle, I could increase L and decrease a to calculate to any desired degree of accuracy. Thus, in principle, I could solve any quantum field theory. Of course, technical issues related to reducing the computation time would remain.

Unfortunately, I do not understand the infinite-volume and continuum limits well and do not know how to place bounds on the errors. Indeed, I believe these limits are not well understood, in general. If one could place bounds on the errors, then

one could probably prove that the limits exist, and thus put quantum field theory on a firm mathematical basis. But to the best of my knowledge, only a limited class of quantum field theories have been proved to exist. Most physically interesting theories are still mathematically dubious.

3.4 Conclusion

I began by noting that the predictive power of the Standard Model is unsatisfactory: No one has successfully calculated quantities in quantum chromodynamics at low energies. My aim has not been to solve quantum chromodynamics, but rather to develop a variational method for calculating physical quantities in quantum field theory. Such a method could, in principle, be applied to quantum chromodynamics.

In Chapter 1 I developed a general method for calculating energy eigenvalues and eigenstates in quantum theories. The Rayleigh-Ritz method, of course, is not new. My original contributions are that my method is systematic, that is capable of achieving arbitrary accuracy; that I quantify errors; and that I optimize the calculation by both selecting basis states and varying nonlinear parameters.

I do not claim that my work is the final word in this area, or even the first: As Wilson pointed out, quantum chemists have been developing variational methods for over sixty years [Wil89]. But I believe that no other variational work in quantum field theory has quantified errors nor attempted to optimize calculations by both selecting basis states and varying nonlinear parameters.

At the end of Chapter 1 I tried to emulate the physical insight that Feynman showed in [Fey87] and many other places. There I asserted that variational methods are not very powerful, being a type of brute force approach. In my opinion, they will never be used to solve quantum chromodynamics, because it is far too complicated. For example, even on a modest lattice with 10 points to a side, quantum chromodynamics has 32000 degrees of freedom. One would need considerably more than 32000 basis states to achieve any reasonable accuracy. Such a calculation is at the limits of current technology, and doubling the size of the lattice increases the number of degrees of freedom by a factor of eight! For quantum field theory the only advantage of variational methods is that they should work, if only one calculates long enough.

No known methods can claim more.

In Chapter 2 I introduced real scalar field theory on a finite lattice, described the weak-coupling basis, and showed how needed quantities could be calculated using that basis. The latter was straightforward but tedious. I could have discussed other types of field theories. But real scalar field theories are relatively simple, providing a testing ground for variational methods free of extraneous complications. I also could have chosen a different basis. The significant idea in Chapter 2 was that one must apply variational methods to finite models of quantum field theory, for example, finite-volume, lattice theories. As I argued at the end of Chapter 1, I believe that all direct applications of variational methods to quantum field theory in the continuum limit are meaningless and doomed to failure.

In Chapter 3 I extended my method to quantum field theory by showing how energy eigenvalues and eigenstates could be related to physical coupling constants and other physical quantities, in particular, bound state energies and scattering amplitudes. Again, much of this work was straightforward but tedious. The connection between energy eigenvalues and eigenstates and Green's functions is, of course, recognized. But, to the best of my knowledge, this connection has never been exploited using variational methods, even though the idea is obvious.

But I was unable to quantify the relation between finite-volume, lattice theories and infinite-volume, continuum theories. Thus I was unable to fully realize my ideas. One could go ahead and calculate anyways, but I do not know how one would interpret the results without any quantitative understanding of the errors. Of course, the relation between finite-volume, lattice theories and infinite-volume, continuum theories is important in itself and has been studied. I am optimistic that this relation can be clarified, thereby completing the realization of my ideas and allowing them to be fully tested.

Lastly, in the process of explaining how variational methods can be used to calculate physical quantities in quantum field theory, I have presented the conceptual structure of quantum field theory in a concrete, albeit nontraditional, way. Doing so has enhanced my understanding of quantum field theory, as I hope it will others.

I had originally hoped to implement my ideas on a computer and to at least reproduced known results for a real scalar field theory in $1+1$ spacetime dimensions

in the perturbative or near-perturbative regime. During most of my research on variational methods, my understanding was not nearly as clear as I hope my presentation here has been. As I developed ideas, I incorporated them into a computer program. But it eventually became clear that my original hope was too optimistic: I was unable to complete a computer program for calculating physical quantities in quantum field theory. In Appendix A I briefly describe the computer program I did write. In Appendix B I present some results for simple quantum mechanical systems obtained using that program.

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Appendix A

Computer Implementation

I implemented many of the ideas in this paper on a computer. In Section A.1 I present an overview of the implementation. In Section A.2 I describe a couple of the more technical algorithms in the implementation.

A.1 Overview of Computer Implementation

I implemented many of the ideas presented in this paper with a computer program. The program accepts commands in a specialized language and performs corresponding actions. Commands can be given in batch mode or interactively. The latter possibility permits the program to be used as an "experimental" tool for studying variational methods. The availability of this tool greatly aided my developing ideas.

One set of commands specify the system under study. There is a command to specify the dimension $d-1 \geq 0$ of the spatial lattice. If the dimension is 0, then the lattice consists of a single point. There are commands to specify the lattice extent L_i and spacing a_i in the ith direction. Note that these may be different in different directions, a slightly more general situation than I described in Chapter 2. And there is a command to specify the (bare) coupling constants $\lambda_\phi, \lambda_0, \lambda_1, \ldots$. Only a finite number of nonzero coupling constants can be specified, that is only polynomial potential densities can be specified. But nonpolynomial potential densities can be

approximated using truncated Taylor expansions. Thus it is possible to specify any of a large class of finite-volume, lattice real scalar field theories.

Another set of commands control the computation. There are commands to specify the sector, that is the total momentum and, if the potential density $V(\phi)$ is even in ϕ, the parity. There is a command to specify the variational parameter μ. And there are commands to control the selection of basis states. One can select all basis states (within the chosen sector) with specified numbers of free particles. Alternatively, one can specify that basis states be selected using the methods of Section 1.3.

Finally, there are many commands for producing or controlling output. These include commands for displaying the current parameters, the approximate eigenvalues and eigenstates, the estimated and "exact" errors, and many types of debugging information. There are various options for controlling the quantity and format of the displayed information.

An innovative feature of the program is that computations are performed only when output is requested, and then only those parts of the computation necessary to the output that have not been performed previously. Furthermore, when parameters are changed, only affected parts of the computation will be redone. Thus one can use the program interactively, changing various parameters and requesting various output, and not have to wait longer than necessary for results.

I wrote the program in C, including the matrix diagonalization routines, which I adapted from [PFTV88]. The program consists of approximatedly 7500 lines of code, including all of the bells, whistles and comments. The C language supports structured programming, recursive functions, complicated data structures, and the dynamical definition of data structures, such as vectors and matrices, with no preset limit to their size. It also results in fairly efficient code.

I wrote the command interpreter portion of the program using YACC and LEX. YACC is a program that generates command parsing routines in, for example, C from a formal specification of the command language grammar. LEX is a program that generates lexical analysis routines in, for example, C from a formal specification of the basic lexical units in the command language. My use of YACC and LEX enabled me to easily add or modify commands, as my ideas and the program developed.

Initially, I wrote the program on an IBM RT PC. Later, when it became available, I transferred the program to a faster Sun SPARCstation 1+. Both machines run versions of UNIX.

I produced the plots in Appendix B using GNUPLOT. This package can produce plots in LaTeX form that can be directly incorporated into LaTeX documents. In producing the plots I was greatly assisted by various filters (GREP, SED, AWK, etc.) available in UNIX.

A.2 Descriptions of Special Algorithms

In this section I describe an algorithm for efficiently calculating the correction functions $\tilde{\Omega}_\ell(Y)$ discussed in Section 2.3. I also discuss a similar algorithm for generating basis states to consider for selection that are likely to have high values, as I discussed in Section 1.3. This material is technical and should be interesting mainly to those wishing to implement my ideas on a computer.

A.2.1 Calculation of Correction Functions $\tilde{\Omega}_\ell(Y)$

We need to calculate correction functions $\tilde{\Omega}_\ell(Y)$ for all basis states Y such that $Y \leq C$ for some selected basis state C. The state Y need not be in the sector under study. A problem is how to generate all such states Y given a list of n selected basis states. In this subsection I present an algorithm for doing so.

If the lattice has N points, then there are N distinct momenta, which we can label $\mathbf{p}_1, \ldots, \mathbf{p}_N$. The order of the momenta is arbitrary but should be fixed.

An arbitrary basis state Y can be generated in a canonical way by starting with the 0-particle state 0, adding $Y_{\mathbf{p}_1}$ free particles with momentum $\mathbf{p}_1$, then adding $Y_{\mathbf{p}_2}$ particles with momentum $\mathbf{p}_2$, and so on. In other words, the particles in Y are added in order of momentum.

We obtain an infinite tree by considering all possible ways that particles can be added in order of momentum starting with the state 0. For example, the node of the tree corresponding to the state 0 has N branches leading from it, one corresponding to adding one particle with any of the N momenta $\mathbf{p}_1, \ldots, \mathbf{p}_N$. The node corresponding

to the state $|\mathbf{p}_{17}\rangle$, consisting of a single particle with momentum $\mathbf{p}_{17}$, has $N-16$ branches leading from it, one corresponding to adding one particle with any of the $N-16$ momenta $\mathbf{p}_{17},\ldots,\mathbf{p}_N$. The root of the tree corresponds to the state 0, and there is a unique node for each possible state. Starting from the root the tree provides a unique path to the node for any given state.

We can generate all states by traversing the tree in depth-first order. In particular, we start with the state 0. If we are at some state Y, we then traverse the subtree under the branch corresponding to adding one particle with momentum $\mathbf{p}_j$, then the $\mathbf{p}_{j+1}$ branch, and so on up to the $\mathbf{p}_N$ branch. Here j is the *leading index* of Y, that is $Y_{\mathbf{p}_j} > 0$ and $Y_{\mathbf{p}_{j+1}} = \cdots = Y_{\mathbf{p}_N} = 0$. The leading index of the state 0 is 1.

We can generate all states Y such that $Y \leq C$ for some selected state C by traversing the tree in depth-first order and pruning all subtrees that contain no selected states. In particular, if Y' is a state in the subtree with root Y, then $Y'_{\mathbf{p}_i} = Y_{\mathbf{p}_i}$ for $1 \leq i < j$, and $Y'_{\mathbf{p}_i} \geq Y_{\mathbf{p}_i}$ for $j \leq i \leq N$, where j is the leading index of Y. We can consider each of the n selected states to determine if any is in the subtree with root Y. If not, then we prune the subtree. We make this determination separately for each visited state Y, although more efficient methods are possible.

In summary, we can generate all states Y such that $Y \leq C$ for some selected state C by traversing a pruned tree of states. This is an $O(n^2)$ computation, assuming the selected states are not sparse. Having done so, for each Y we can calculate $\tilde{\Omega}_\ell(Y)$ by looping over all selected states C.

A.2.2 Generation of States Likely To Have High Values

In Section 1.3 I mentioned that the number of unselected basis states connected by the hamiltonian to at least one selected basis state can be large. Thus it is not always practical to consider all such unselected states for selection. In this subsection I describe an algorithm for generating basis states to consider for selection that are likely to have high values.

One key idea is as follows: We can think of each basis state A as a point in an N-dimensional lattice. The N components of the point are the N integers $A_{\mathbf{p}_1},\ldots,A_{\mathbf{p}_N} \geq 0$. In fact, the state lattice separates into disjoint sets corresponding

to different sectors, but never mind this technical complication for now. We want to locate those states with the highest values. I call the state lattice a "gold mine," the gold being the valuable states. We want to "mine," that is select, the valuable states. It is prudent to first "explore," that is estimate, the values of many states before deciding which states to mine. It is plausible that states close to each other in the lattice have similar values. If we find a high-value state, then we should explore the "vein" of nearby states.

My algorithm is a combination of the gold mine idea and the state tree idea of the previous subsection. In particular, we first explore the state 0 at the root of the tree. After exploring some state A, we might want to explore the vein leading from A, that is the states immediately under A in the tree. The initial estimate of the "yield" of this vein is the value of A. We do not traverse the tree in any fixed order; rather we explore many veins at once. At any given time we explore the next state in the vein with the current highest estimated yield. Whenever we explore a state in a vein, we update our estimate of the yield of the vein using the value of the state just explored. For example, the new estimated yield of the vein is a weighted average of the old estimated yield and the value of the state just explored. Thus which vein has the highest estimated yield changes. We continuing exploring states until we have explored all states with value, or until we have explored a sufficient number of states. From the explored states, we select some with the highest values.

To implement these ideas we maintain a priority queue of states with their values. A priority queue is a "largest-in, first-out" queue. As we explore states, we add them with their values to the queue. When we are done exploring, we can get the states with the highest values immediately from the queue.

We also maintain a priority queue of veins with their estimated yields. In particular, the vein associated with the state A is the set of $N-j+1$ states that result from adding to A one particle with any of the $N-j+1$ momenta $\mathbf{p}_j,\ldots,\mathbf{p}_N$. Here j is the leading index of A. We explore the states in a vein in some fixed order. An entry in the vein priority queue specifies the next state in the vein to be explored. Whenever we explore a state, we add the vein associated with that state to the vein priority queue.

We start by exploring the state 0, adding it to the state priority queue, and

adding the associated vein to the vein priority queue. Whenever we get the vein with the current highest estimated yield, we delete it from the vein priority queue. We then explore the next state in the vein. If there are still unexplored states in the vein, we update its estimated yield and add it again to the vein priority queue.

The remarks above describe the main features of my algorithm, but a few technical points remain. First, it is reasonable to explore the states in a vein in the order $\mathbf{p}_j, \ldots, \mathbf{p}_N$ such that $\omega_{\mathbf{p}_j} \leq \cdots \leq \omega_{\mathbf{p}_N}$, where j is the leading index of the original state. In other words, we explore states with low free energy first.

Second, the only states that have (estimated) value are those in the sector under study, and of these only those connected by the hamiltonian to at least one selected state. If we explore a state with no value, then we immediately explore the state in its vein with value, the rule above for ordering states in a vein notwithstanding. If there is no such state in the vein (because all of the states in the vein have the wrong total momentum or wrong parity), then we immediately explore the first state in the vein. And so on recursively. The initial estimated yield of all veins we open in this process is the value of the first state with value we find. If a state has no value, we do not add it to the state priority queue, but we do add the associated vein to the vein priority queue.

Third, the value of a selected state u_i is $|\langle u_i|e_k\rangle|^2 \approx |\langle u_i|e_k^{(n)}\rangle|^2$. If we want to increase the number of selected states by adding unselected states, then currently selected states should not be added to the state priority queue when they are explored: We simply retain all currently selected states and then add unselected states from the queue. Alternatively, if we want to reconsider the currently selected states, then these should be added to the state priority queue and treated on an equal footing with currently unselected states: We select anew states from the queue.

The algorithm I have described above is a reasonable method for efficiently generating states to consider for selection likely to have high values.

Appendix B

Results for Quantum Mechanics

Here I present a sample of the results of applying the method to simple quantum mechanical systems. In Section B.1 I examine the correctness of the method and its implementation. In Section B.2 I study the behavior of the algorithms with various choices of basis states and variational parameters.

B.1 Tests of Method Correctness

In this section I describe ways of testing the correctness of the method and its computer implementation and present the results of a sample of those tests.

There are many ways of testing the correctness of the method and its computer implementation. For example, we can verify by direct multiplication that the n approximate eigenvalues $\epsilon_i^{(n)}$ and eigenstates $e_i^{(n)}$ of H are exact eigenvalues and eigenstates of the $n \times n$ matrix H_n. We can also verify that the eigenstates are orthonormal. Doing so tests the correctness of the matrix diagonalization routines, but does not guarantee that the matrix elements $\langle u_i|H|u_j\rangle$ are correct, that is that we are solving the system we think we are.[1]

A better type of test is to compare the results of the program with known

[1] While developing the program, I encountered such an error. The program produced plausible results that were just inaccurate enough and inconsistent enough to arouse suspicion. It turned out that a few of the more complicated matrix elements were slightly incorrect. The error occurred only for lattices with more than one point and potential densities with at least a ϕ^4 term.

results. Since the program produces approximate results, such comparisons make sense only if we estimate the errors, as described in Section 1.2. The correctness of the program is verified if the known results fall within the estimated error limits. Such tests can fail if the matrix elements are incorrect, if the matrix diagonalization routines are incorrect, or if the error estimates are overly optimistic. The latter possibility can occur, for example, if the variance calculations are incorrect. Thus such tests can provide very strong confidence in the method and its implementation.

There are many known results at our disposal. For example, we can consider a theory of free particles with mass m on an arbitrary lattice, defined by the potential density $V(\phi) = \frac{1}{2}m^2\lambda_\phi\phi^2 + \lambda_0$. It is convenient to choose $\lambda_0 = -\frac{1}{2}L^{-(d-1)}\sum_{\mathbf{p}}\omega_{\mathbf{p}}$ such that the ground state energy is 0, where $\omega_{\mathbf{p}}$ is given by Equation (2.27). Then each eigenstate is a free particle state $|A\rangle$ with energy $\sum_{\mathbf{p}} A_{\mathbf{p}}\omega_{\mathbf{p}}$. Such theories are nontrivial if we perform calculations using a variational parameter $\mu \neq m$.

The Montroll group [HM75, HMM78] extensively studied systems consisting of a single or a pair of coupled oscillators with quartic potentials. Unfortunately, their two-oscillator systems cannot be cast into the form of a real scalar field theory on a two-point lattice.

It is possible to generate a wide class of single-oscillator systems with polynomial potentials such that the ground state and ground state energy are exactly known.[2] The trick is to first specify the ground state wave function

$$\psi_0(q) \sim e^{P(q)}, \tag{B.1}$$

where $P(q)$ is a polynomial in q that is bounded above. Then we can solve for the potential $V(q)$ and ground state energy ε_0 such that

$$H|\psi_0\rangle = \left[-\frac{1}{2}\frac{d^2}{dq^2} + V(q)\right]|\psi_0\rangle = \varepsilon_0|\psi_0\rangle. \tag{B.2}$$

A system consisting of a single oscillator with a potential hole of the modified Pöschl-Teller type can be solved exactly [Flü71]. It is defined by the potential

$$V(q) = -\alpha^2\frac{\lambda(\lambda-1)}{\cosh^2\alpha q}, \tag{B.3}$$

[2] I am grateful to Ivan Otero for showing me this trick.

where λ and α are coupling constants. The potential is nonpolynomial, but it can be approximated by a truncated Taylor series with many terms.

We can generalize any of the solvable one-oscillator systems discussed above to essentially solvable systems on an arbitrary lattice: We simply use the same potential and choose a large enough lattice spacing a so that the oscillators at each lattice point are weakly coupled to each other, that is so that the coupling constants $\lambda_0, \lambda_1, \ldots$ are strong. We can calculate approximate, but accurate, energy eigenvalues by treating as a small perturbation the piece H_{con} of the hamiltonian that connects neighboring lattice points, as I discussed in Section 2.2. Such systems in the strong-coupling limit provide a good test of the method, which we expect to work best in the weak-coupling limit.

Lastly, we can test the method using unsolved systems. We simply solve the system repeatedly by running the program with many different choices of basis states and the variational parameter μ. If all results are consistent to within the estimated error bounds, then our confidence in the method increases.

In particular, if we choose a good value for μ and select sufficiently many basis states, then the program can compute eigenvalues and eigenstates that are "exact" within the precision of the machine (approximately 15 significant figures). These eigenvalues and eigenstates are more precise than other published numerical results and can serve as benchmarks against which to compare other less accurate computations with the program.

The method and its computer implementation have passed all tests that I have run. In order to give the flavor of these tests, I will focus on just one system and present the results of tests using that system.

In particular, consider the single oscillator system defined by the hamiltonian

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}q^2 + 1000\,q^4, \tag{B.4}$$

which was studied by the Montroll group [HM75]. In Table B.1 I compare the lowest few eigenvalues they present with those produced by the computer implementation. The computed eigenvalues agree with those in [HM75] but are far more precise. In what follows, I treat these computed values as being "exact."

An approximate eigenvalue $\varepsilon_k^{(n)}$ produced by the method is an upper bound

	Montroll Group	Computer Implementation
ε_0	6.694 220 85	6.694 220 850 504 03
ε_1	23.972 206 1	23.972 206 056 383 1
ε_2	47.017 338 7	47.017 338 732 427 7
ε_3	73.419 114 0	73.419 113 844 530 5
ε_4	102.516 157	102.516 157 134 231
ε_5	133.876 891	133.876 891 218 831
ε_6	167.212 258	167.212 258 193 636
ε_7	202.311 20	202.311 199 675 512
ε_8	239.011 58	239.011 577 550 546

Table B.1: Comparison between the lowest few eigenvalues ε_k given by the Montroll group [HM75] and those produced by the computer implementation for the one-oscillator system defined by $H = \frac{1}{2}p^2 + \frac{1}{2}q^2 + 1000\,q^4$. In the computer calculation $\mu = 50$ and the first $n = 25$ basis states with the correct parity are selected: states with $0, 2, \ldots, 48$ particles for even parity and states with $1, 3, \ldots, 49$ particles for odd parity. The estimated errors are all below the precision of the machine.

to the exact eigenvalue ε_k. As I discussed in Section 1.2, the Kato theorem provides a lower bound to the eigenvalue or, equivalently, a bound on the error $\eta_k^{(n)} = |\varepsilon_k^{(n)} - \varepsilon_k|$. Since we know the first few eigenvalues (to 15 significant figures), we can calculate the actual eigenvalue error. If the method and its implementation are correct, the actual error should be less than the estimated error provided by the Kato theorem. In Figure B.1 I compare the estimated and actual errors for the lowest eigenvalue ε_0. The approximate eigenvalues are computed using various numbers of selected basis states and values for the variational parameter μ. In all cases, the actual eigenvalue error is less than the corresponding estimated error.

The Kato theorem also provides a bound on the eigenstate error $\zeta_k^{(n)}$ between the approximate eigenstate $e_k^{(n)}$ and the corresponding exact eigenstate e_k, as I discussed in Section 1.2. If we select enough basis states, then we can treat the eigenstates computed by the program as "exact," although I know of no published results with which to compare these. Thus we can calculate the actual eigenstate error between an approximate eigenstate, computed using a small number n of selected basis states or a poor choice of μ, and the exact eigenstate. The actual eigenstate error should be less than the estimated eigenstate error provided by the Kato theorem.

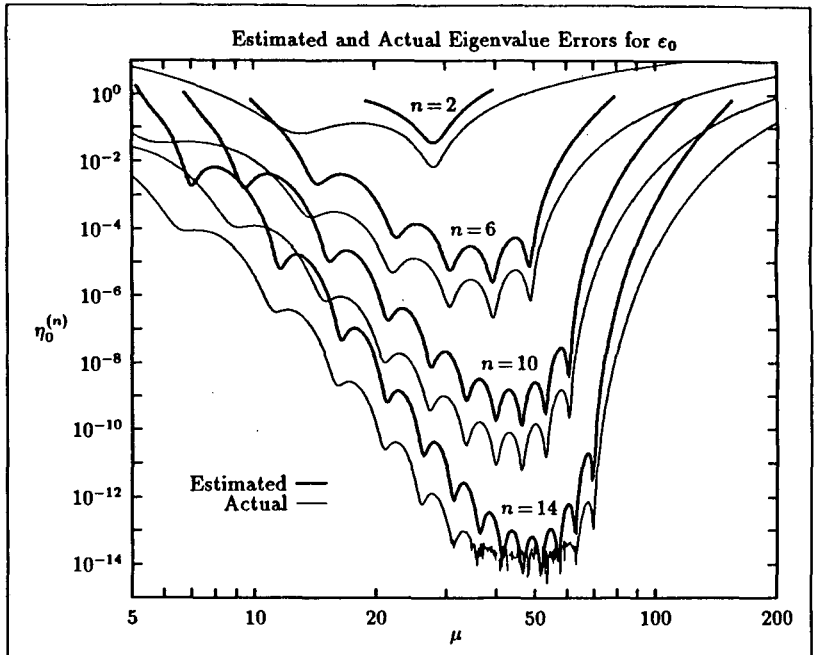

Figure B.1: Comparison between the estimated and the actual errors $\eta_0^{(n)}$ for the lowest eigenvalue $\varepsilon_0 = 6.694\,220\,850\,504\,03\ldots$ for the one-oscillator system defined by $H = \frac{1}{2}p^2 + \frac{1}{2}q^2 + 1000\,q^4$. The selected basis states are the first n states with $0, 2, \ldots$ particles, where n is 2, 6, 10 or 14. Various values of the variational parameter μ are used. Each pair of estimated and actual points represents a single variational calculation. The estimated errors are larger than the actual errors by an order of magnitude or so, but otherwise seem to parallel the actual errors. Note that estimated errors are not shown when they are so large as to be unreliable. Also note that the noise at the bottom of the $n = 14$ curve for the actual errors is due to the limited precision of the machine (15 significant figures).

In Figure B.2 I compare the estimated and actual errors for the lowest eigenstate e_0. The approximate eigenstates are computed using the same numbers of selected basis states and values for the variational parameter μ as in Figure B.1.

Note that approximate and exact eigenstates can be compared easily only if they are expressed in terms of the same basis, that is in terms of bases with the same value of μ. Thus it is necessary to recompute the exact eigenstate for each value of μ plotted: Figure B.2 represents a lot of computations!

B.2 Behavior of Method

In this section I present the results of applying the method to some interesting quantum mechanical systems. In particular, I show how well the method selects basis states and chooses the variational parameter μ.

B.2.1 Selection of Basis States: Weakly-Coupled System

Consider a theory of free particles with mass $m = 1$ in $1+1$ spacetime dimensions defined by the potential density $V(\phi) = \frac{1}{2}\phi^2 + \lambda_0$. Let the lattice have $N = 10$ points with spacing $a = \pi/50$. Thus the lattice size is $L = \pi/5$. We can choose λ_0 such that the vacuum energy is 0.

The theory describes free particles with any of 10 possible momenta, whose energies are given by Equation (2.27). All nonzero momenta are large compared to the mass $m = 1$ (Table B.2).

If we choose $\mu = m = 1$, then each energy eigenstate is a basis state with energy equal to the total energy of its constituent particles. Particles with nonzero momenta have much larger energies than particles with zero momenta. Thus in the zero total momentum, even parity sector, the lowest few energy eigenstates consist of only zero momentum particles (Table B.3).

If we use a basis with $\mu = 2$, then each eigenstate is no longer a single basis state, but rather a superposition of basis states. We can view the theory as describing fictitious free particles with mass $\mu = 2$, except there is a weak quadratic self-coupling, which effectively changes the mass. In what follows, I study this theory

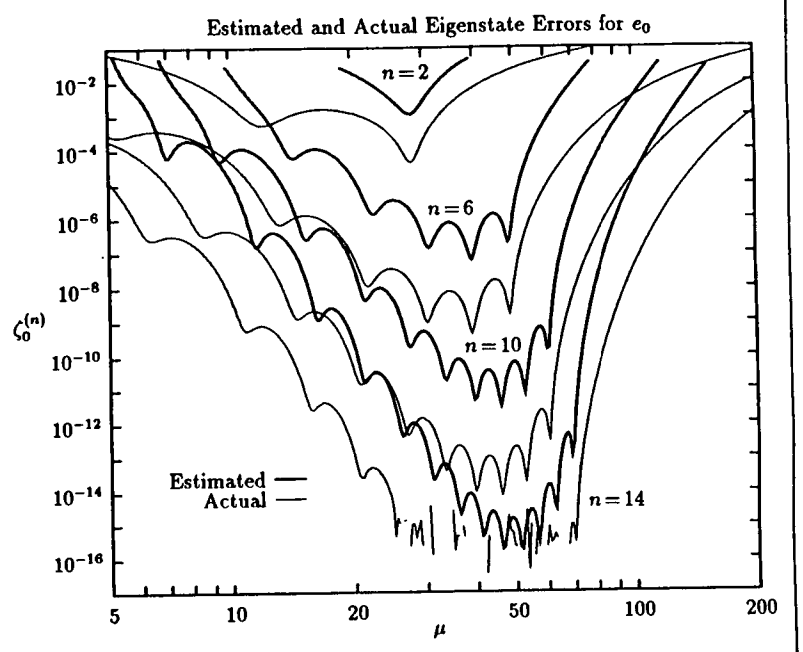

Figure B.2: Comparison between the estimated and the actual errors $\zeta_0^{(n)}$ for the lowest eigenstate e_0 for the one-oscillator system defined by $H = \frac{1}{2}p^2 + \frac{1}{2}q^2 + 1000\,q^4$. The selected basis states are the first n states with $0, 2, \ldots$ particles, where n is 2, 6, 10 or 14. Various values of the variational parameter μ are used. Each pair of estimated and actual points represents a single variational calculation. The estimated errors are larger than the actual errors by an order of magnitude or so, but otherwise seem to parallel the actual errors. Note that estimated errors are not shown when they are so large as to be unreliable. Also note that the noise at the bottom of the $n = 14$ curve for the actual errors is due to the limited precision of the machine (15 significant figures). Finally, note the similarity between the curves for the estimated eigenstate errors and the corresponding curves for the estimated eigenvalue errors in Figure B.1: The similarity occurs in general.

p	ω_p ($\mu = 1$)	ω_p ($\mu = 2$)
0	1.000 000	2.000 000
±10	9.887 017	10.037 58
±20	18.736 49	18.816 37
±30	25.771 21	25.829 35
±40	30.289 58	30.339 06
50	31.846 69	31.893 75

Table B.2: Free particle momenta and energies for the weakly-coupled system in $1+1$ spacetime dimensions defined by the potential density $V(\phi) = \frac{1}{2}\phi^2 + \lambda_0$. The lattice has $N = 10$ points with spacing $a = \pi/50$. The $\mu = 1$ energies are the actual energies; the $\mu = 2$ energies are fictitious.

using $\mu = 2$.

Equation (2.27) gives the energies the fictitious particles would have if their mass were $\mu = 2$. Note that the free particle energies are roughly the same for $\mu = 1$ and $\mu = 2$ (Table B.2).

Although energy eigenstates are not $\mu = 2$ basis states, we expect the lowest eigenstates to be superpositions of basis states consisting of primarily zero or low momentum particles. But the number of distinct basis states in the zero total momentum, even parity sector grows rapidly as the number of particles increases. If the basis state selection algorithm works well, then it should efficiently find the valuable states consisting of zero or low momentum particles amongst all the basis states in the sector.

In particular, I begin by selecting just the 0-particle state. The program then selects additional basis states so as to improve the approximation to the ground state. The attached tables and figures describe the weakly-coupled system, the selection process, and the results thereof.

Note that the same kinds of tests can be done with a strongly-coupled theory. For example, consider a generalization of the single oscillator system studied by the Montroll group. In particular, consider a theory in $1+1$ spacetime dimensions defined by the potential density $V(\phi) = \frac{1}{2}\phi^2 + 1000\,\phi^4$. Let the lattice have $N = 10$ points

State	Energy	State	Energy
0	0	14(0)	14
2(0)	2	16(0)	16
4(0)	4	18(0)	18
6(0)	6	(10)+(−10)	19.774 03
8(0)	8	20(0)	20
10(0)	10	2(0)+(10)+(−10)	21.774 03
12(0)	12	22(0)	22

Table B.3: Lowest few energy eigenstates and eigenvalues in the zero momentum, even parity sector for the weakly-coupled system in $1 + 1$ spacetime dimensions defined by the potential density $V(\phi) = \frac{1}{2}\phi^2 + \lambda_0$. The lattice has $N = 10$ points with spacing $a = \pi/50$. Here $\lambda_0 = -160.9178\ldots$ is chosen such that the vacuum energy is 0. The notation 2(0)(10)(−10) means 2 particles with momentum 0, 1 particle with momentum 10, and 1 particle with momentum −10.

with spacing $a = \pi/5$, and hence the lattice size is $L = 2\pi$. Thus all of the momenta are small compared to a typical energy $\mu = 50$. In this case, all of the free particles energies are roughly equal. States with the fewest particles (and hence lowest free energies) are selected first, almost independently of their energies. One finds that the algorithm works as anticipated for a strongly-coupled theory.

Pass	Selected States	Acceptable States	Explored States	Maximum Veins
1	1			
2	2	6	7	1
3	3	11	2	3
4	5	16	7	3
5	8	25	33	6
6	12	37	73	9
7	18	45	74	12
8	27	63	35	18
9	41	86	293	25
10	62	117	237	38
11	93	161	855	54
12	140	216	6509	76
13	210	300	10545	112
14	315	409	17383	164
15	473	550	28237	233

Table B.4: Summary of the basis state selection process in the zero momentum, even parity sector for the weakly-coupled system. The $\mu = 2$ basis is used. In the first pass only the 0-particle state is selected. In each successive pass all currently selected states are retained and other states with the highest estimated values are also selected. All values are relative to the ground state. "Selected States" is the number of states selected; "Acceptable States" is the number of states considered that are in the proper sector and connected by the hamiltonian to at least one currently selected state; and "Explored States" is the total number of states considered. All three numbers include currently selected states. In each pass, all possible acceptable states were explored. "Maximum Veins" is the maximum number of open veins in the vein priority queue at any time during the pass.

Particles	Selected States	Possible States	Particles	Selected States	Possible States
0	1	1	16	34	204347
2	6	6	18	28	468754
4	21	73	20	24	1001603
6	56	504	22	20	2016144
8	81	2438	24	14	3856892
10	69	9252	26	10	7060984
12	58	29414	28	7	12440668
14	44	81752			

Table B.5: Number of selected and possible basis states with given numbers of particles in the zero total momentum, even parity sector for the weakly-coupled system. The selected states are the $n = 473$ states selected in pass 15 of the selection process summarized in Table B.4.

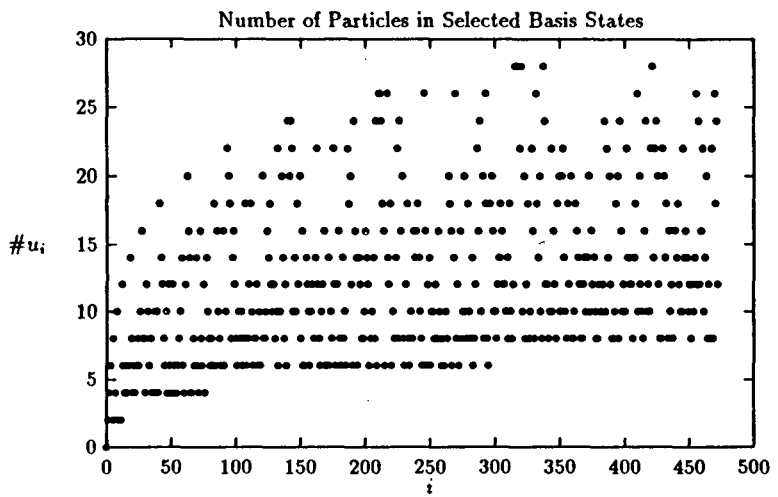

Figure B.3: Numbers of particles $\#u_i$ in selected basis states u_i in the zero total momentum, even parity sector for the weakly-coupled system. The selected states are the $n = 473$ states selected in pass 15 of the selection process summarized in Table B.4. Basis states are plotted from left to right in the order in which they were selected. Note the tendency for states selected later to have more particles. But states with many particles are underrepresented, considering the possible number of such states.

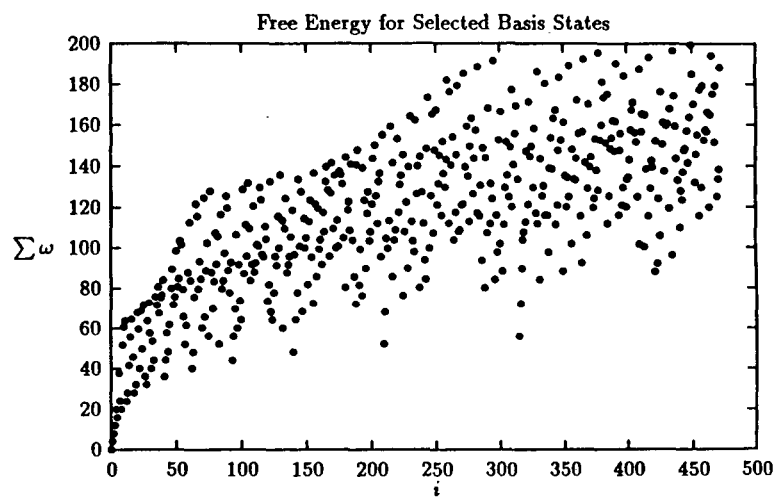

Figure B.4: Free energies $\sum_{\mathbf{p}} u_{i\mathbf{p}}\omega_{\mathbf{p}}$ of selected basis states u_i in the zero total momentum, even parity sector for the weakly-coupled system. Free energies are for particles with mass $\mu = 2$. The selected states are the $n = 473$ states selected in pass 15 of the selection process summarized in Table B.4. Basis states are plotted from left to right in the order in which they were selected. Note the tendency for states selected later to have higher free energies. Also note that all of the free energies are relatively modest compared to the energy of a few particle with momentum 50, that is energy ~ 30.

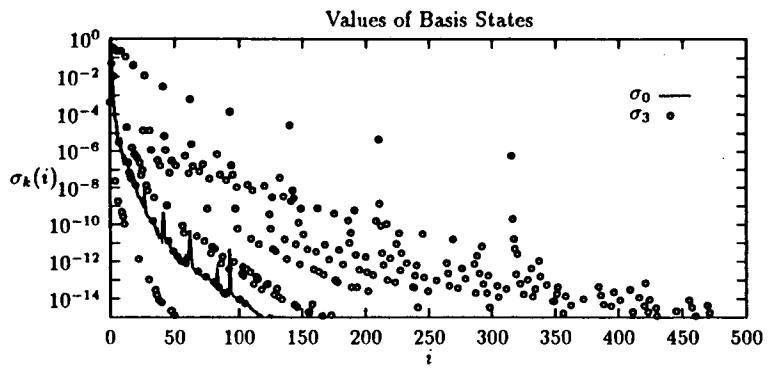

Figure B.5: Values $\sigma_k(i) = |\langle u_i | e_k^{(n)} \rangle|^2$ for the selected basis states u_i relative to the approximate eigenstate $e_k^{(n)}$ in the zero total momentum, even parity sector for the weakly-coupled system. The selected states are the $n = 473$ states selected in pass 15 of the selection process summarized in Table B.4. Basis states are plotted from left to right in the order in which they were selected. The values for the ground state e_0 decrease almost monotonically, indicating that the basis state selection algorithm is working well. The values for the third excited state e_3 in the sector also tend to decrease, but the effect is not as strong, since no attempt was made to select basis states with high value relative to e_3.

B.2.2 Choice of Variational Parameter: Anharmonic Oscillator

In order to study the effect of varying μ, consider a single oscillator system defined by the potential

$$V(q) = q^2 + q^4 + q^6. \tag{B.5}$$

We can find approximate eigenstates in the even parity sector using the first $n = 50$ states with $0, 2, \ldots, 98$ particles and various choices of μ. If my concepts in Section 1.3 are correct, then we expect that 1) $\ln |\langle u_i | e_k^{(n)} \rangle|^2$ is a linear function of i for fixed k, 2) the values of μ that produce the smallest errors are those that result in the steepest slope, and 3) for large enough i we get the same slope for any i and fixed μ. The attached figures show some of this behavior.

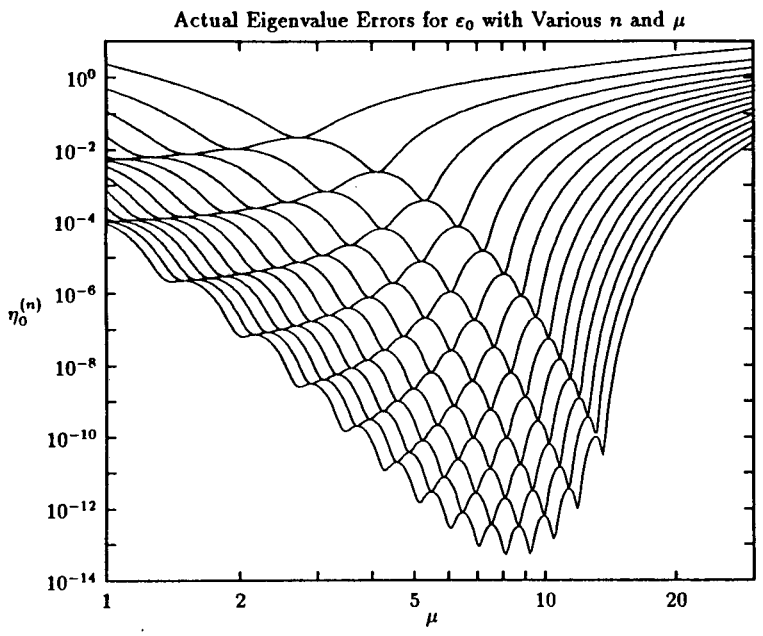

Figure B.6: Actual eigenvalue errors $\eta_0^{(n)}$ for the lowest eigenvalue ϵ_0 in the even parity sector for the one-oscillator system defined by $V(q) = q^2 + q^4 + q^6$. The selected basis states are the first n states with $0, 2, \ldots$ particles, where n is $1, \ldots, 15$. Various values of the variational parameter μ are used. Though not labeled, each curve for fixed n is easily recognized, because Rayleigh-Ritz approximate eigenvalues decrease monotonically as basis states are added, hence so do actual eigenvalue errors: Curves for different n do not cross. Observe that the best values for the variational parameter cluster around $\mu = 10$. The "stacked arches" appearance of this plot seems to be typical, at least for one oscillator systems. In more complicated systems analogous periodic behavior is observed. Note that each additional basis state reduces the error by an order of magnitude, at least in the vicinity of $\mu = 10$.

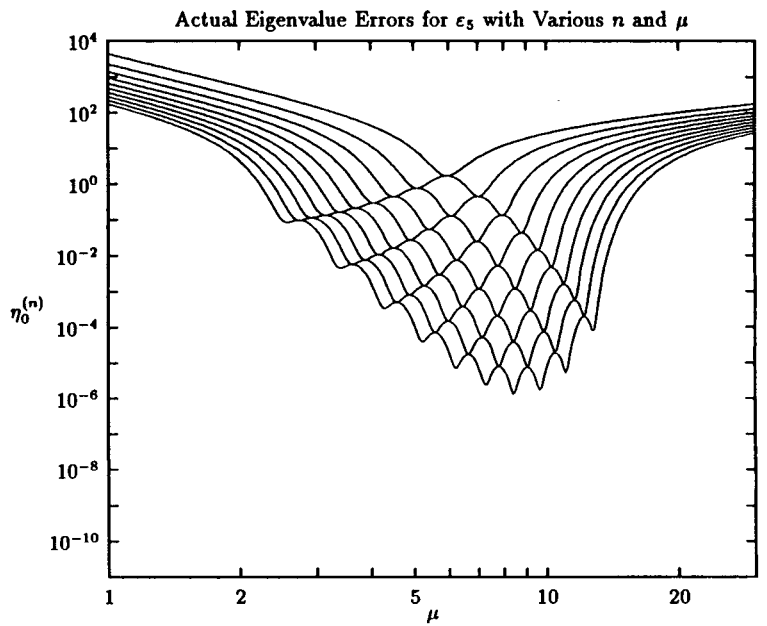

Figure B.7: Actual eigenvalue errors $\eta_5^{(n)}$ for the fifth excited eigenvalue ϵ_5 in the even parity sector for the one-oscillator system defined by $V(q) = q^2 + q^4 + q^6$. The selected basis states are the first n states with $0, 2, \ldots$ particles, where n is $6, \ldots, 15$. Various values of the variational parameter μ are used. Though not labeled, each curve for fixed n is easily recognized, because Rayleigh-Ritz approximate eigenvalues decrease monotonically as basis states are added, hence so do actual eigenvalue errors: Curves for different n do not cross. Observe that the best values for the variational parameter cluster around $\mu = 10$, the same value as for the ground state.

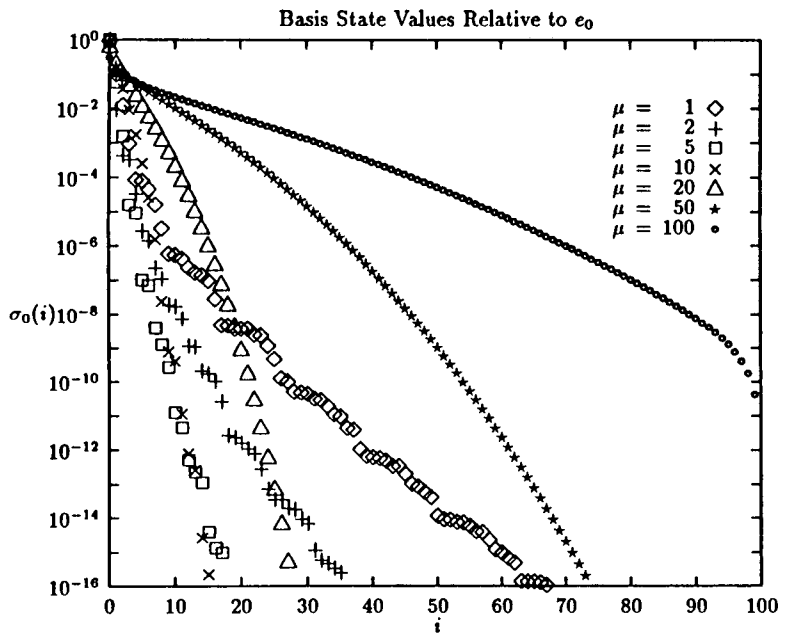

Figure B.8: Approximate basis state values $\sigma_0(i) = |\langle u_i|e_0^{(n)}\rangle|^2$ relative to the ground state e_0 in the even parity sector for the one-oscillator system defined by $V(q) = q^2 + q^4 + q^6$. Various values for the variational parameter μ are chosen. The selected basis states are the first $n = 100$ states with $0, 2, \ldots$ particles. Basis states are ordered from left to right in decreasing value *independently for each* μ. Note that the values decrease roughly exponential for each choice of μ. It is clear that $\mu = 5$ or 10 are the best choices. Observe how the slope of the $\mu = 50$ and $\mu = 100$ curves approach that of the $\mu = 10$ curve.

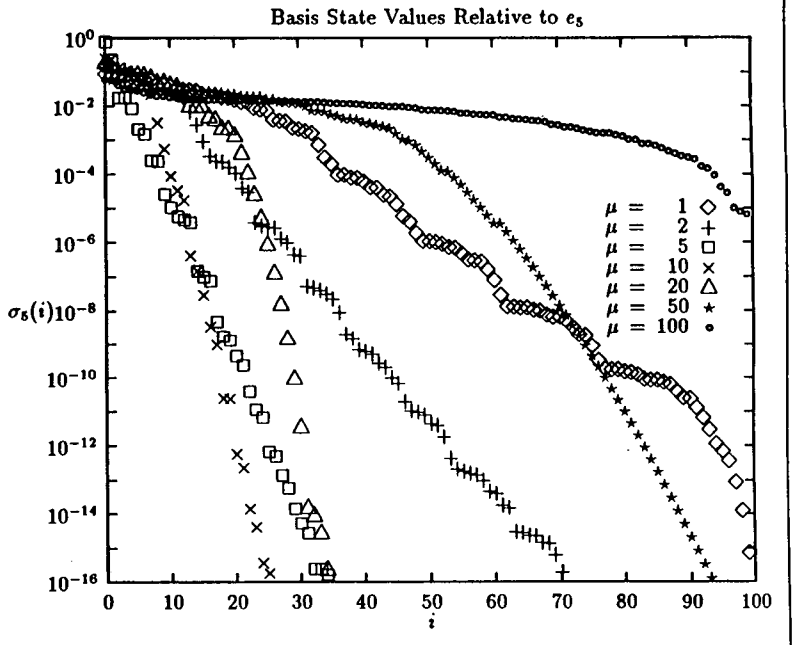

Figure B.9: Approximate basis state values $\sigma_5(i) = |\langle u_i|e_5^{(n)}\rangle|^2$ relative to the fifth excited state e_5 in the even parity sector for the one-oscillator system defined by $V(q) = q^2 + q^4 + q^6$. Various values for the variational parameter μ are chosen. The selected basis states are the first $n = 100$ states with $0, 2, \ldots$ particles. Basis states are ordered from left to right in decreasing value *independently for each* μ. Note that the values decrease roughly exponential for each choice of μ. It is clear that $\mu = 10$ is the best choice, but $\mu = 5$ and $\mu = 20$ are almost as good. Observe how the slope of the $\mu = 50$ curve approaches that of the $\mu = 10$ curve.

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