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Hamiltonians, Path Integrals and A New Renormalization Group*

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ABSTRACT

New non-perturbative methods for dealing with Hamiltonian systems are introduced. The derivation of these methods requires identities for rewriting exponentials of sums of operators which are different from the usual Campbell-Hausdorff formula. These identities allow one to derive approximations to $e^{-\delta H}$ which are correct to higher order in δ and which contain fewer terms than the Campbell-Hausdorff formula. This allows one to generate path-integral actions which are more accurate for finite size steps in time and which can be exploited to improve the rate of convergence of Monte-Carlo calculations. To show that these methods allow one to include effects which show up in the stationary phase approximation to the path integral, e.g. instantons, solitons, etc., I not only derive the connection between the Hamiltonian and path-integral formalism but the relationship between a specific stationary-phase approximation and the corresponding Hamiltonian calculation. My focus, however, is the direct application of these new identities to the study of non-perturbative Hamiltonian dynamics. I show that these methods are easier to apply and give better results than those based upon the naive t-expansion, block-mean field or real-space renormalization ideas. Comparison of the these older methods with the computational tools introduced in this paper are discussed in the context of simple examples. It is shown that the new methods allow one to extrapolate answers to finite t without the use of Padé approximants.

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1. Introduction

This paper develops new, Hamiltonian based, non-perturbative calculational methods for studying quantum mechanical systems. These techniques are simpler to implement, are more accurate and avoid problems encountered in previous methods such as the Hamiltonian real-space renormalization group [3] and t-expansion [1]. What is more, these methods make manifest the relationship between a specific stationary phase approximation to the path-integral and a specific Hamiltonian calculation, thus opening the door to the incorporation of instantons, etc. into Hamiltonian approximation schemes.

The key to establishing the relationship between path-integral and Hamiltonian approximations is a better understanding of the conventional derivation of the path-integral and the the approximations upon which it is based. It is crucial to understand the operator foundation of Feynman's rewriting of $e^{-\delta H}$ as a product of simpler factors and the way one can systematically improve upon this approximation. In what follows I investigate this question, provide one possible extension of these ideas and use the resulting formalism to establish the correspondence between a given stationary-phase approximation to the path-integral and a specific Hamiltonian calculation [6]. While these results are interesting, the real payoff lies in the fact that these better approximation methods can be directly utilized in Hamiltonian calculations without reference to path-integral methods. This is especially true in the case of lattice spin-systems, where they lead to a new formulation of mean-field and block mean-field approximations and a new approach to the Hamiltonian real-space renormalization-group. It will become apparent that these computational techniques draw upon ideas related to both the t-expansion and Hamiltonian renormalization-group and in order to keep this paper relatively self-contained I will review the necessary concepts.

Since both the Euclidean path-integral and t-expansion study matrix elements of $e^{-\delta H}$ from different points of view, I begin with a short review of the both techniques. The derivation of the path-integral from a Hamiltonian leads naturally to the question of the best way to approximate $e^{-\delta H}$ for small δ. Since this question is important to a proper understanding of the path-integral and peculiarities of the t-expansion, the review is followed with a discussion of just this point. After discussing general methods for improving upon Feynman's approach I apply the improved approximation to simple quantum systems; in particular, the harmonic and anharmonic oscillator. This discussion shows that if one works at finite values of δ, as one must in the Monte-Carlo approach to evaluating the path-integral, then these improved approximations greatly increase the accuracy of the calculation. As part of this analysis I show that there are two sources of inaccuracy in calculations

of this type, the first related to the specific approximation used for of $e^{-\delta H}$ and the second to the quality of the trial wave-function one starts from. I conclude with a discussion of methods for improving upon the starting wave-function.

These discussions not only lay the foundation for the connecting these ideas to the stationary-phase approximation to the path-integral but they provide a foundation for the Hamiltonian renormalization-group method to be discussed at the end of the paper. After applying these ideas to simple quantum systems I apply them to a more complicated lattice spin system in order to show the rich set of tools this approximation technique provides. I begin with the simplest application of these ideas and show the ways in which they can be extended. As in the case of the simple quantum mechanical system one must discuss both the approximation to $e^{-\delta H}$ being adopted and the way to choose a wave-function in which to evaluate this operator. This brings us naturally to a discussion of the way in which mean-field and renormalization-group concepts come into the approximation scheme.

While this paper is lengthy it only scratches the surface of what can be done and I only touch upon many of the topics. The conclusion of this paper discusses unsolved problems and work currently in progress.

2. The t-Expansion Revisited

The starting point for the t-expansion is the observation that in the limit $t \to \infty$ the state

$$|\Psi(t)\rangle = \frac{e^{-tH/2}}{\sqrt{\langle\Psi| e^{-tH} |\Psi\rangle}} |\Psi\rangle \tag{2.1}$$

converges to the lowest eigenstate of the H with which it has a non-vanishing overlap. In particular, if $\langle\Psi|\Psi_0\rangle \neq 0$, where $|\Psi_0\rangle$ is the ground-state of H, then

$$\mathcal{E}(t) = \langle\Psi(t)| H |\Psi(t)\rangle \tag{2.2}$$

converges to the ground-state energy. Since

$$\mathcal{E}(t) = -\frac{d}{dt} \ln(Z(t)), \tag{2.3}$$

where $Z(t)$ is

$$Z(t) = \langle\Psi| e^{-tH} |\Psi\rangle, \tag{2.4}$$

computing the ground-state energy of H is the same as computing the large t behavior of $Z(t)$. Although an accurate computation of the exact ground-state

energy is the eventual goal, it is important to note that interesting results can be obtained without taking $t \to \infty$. This is because an accurate computation of $\mathcal{E}(t)$ provides an upper bound on the ground-state energy for any value of t.

The basic approach of the naive t-expansion is to expand e^{-tH} as a Taylor series in t, compute the various operator expectation values and reconstruct the large t behavior of $Z(t)$ or $\mathcal{E}(t)$ by means of Padé approximants or by fitting the series to sums of decreasing exponentials. Computations done for lattice spin systems and lattice gauge theories show that low-order series in t produce fairly accurate results for the ground-state energy density and mass gaps. One problem with the t-expansion is that these same calculations indicate that highly accurate computations require going to high order in t. Not surprisingly, t-expansion calculations become increasingly difficult in higher order and although many computations eventually simplify dramatically, there is no systematic way of recognizing cancellations at an early stage. Another problem is that Padé approximants or exponential fits to $Z(t)$ introduce unknown errors and a certain arbitrariness remains in the process which makes it difficult to estimate the accuracy of a given calculation.

Part of the motivation for the present work is to find methods to compute $Z(t)$ which exhibit cancellations at an early stage and automatically resum large parts of the Taylor series, thereby reducing or eliminating the need for Padé approximants. Since the path-integral is an alternative way of computing $Z(t)$ it is natural to reexamine the steps which go into the derivation of the formalism to see which ideas can be adapted to the Hamiltonian approach.

2.1 Concerning The Path-Integral

Consider a system defined by two operators P and X which satisfy the canonical commutation relation

$$[X, P] = i \tag{2.5}$$

and a Hamiltonian of the form

$$H = \frac{P^2}{2m} + V(X). \tag{2.6}$$

To maintain contact with the t-expansion I will focus on computing matrix elements of the operator

$$C(t) = e^{-tH} \tag{2.7}$$

The usual derivation of a path integral representation for a matrix element of this

operator begins by rewriting it as

$$\langle\psi|\, C(t)\,|\psi\rangle = \langle\psi|\, C(\delta)^n\,|\psi\rangle\,, \tag{2.8}$$

where $\delta = t/n$ and $|\psi\rangle$ is some normalized state, and noting that

$$C(\delta) \approx e^{-\delta P^2/2m}\, e^{-\delta V(X))}\, e^{\mathcal{O}(\delta^2)} \tag{2.9}$$

Because terms of order δ^2 can be ignored in the limit $\delta \to 0$, the factor $e^{\mathcal{O}(\delta^2)}$ is set to unity. Rewriting Eq. (2.8) by inserting a complete set of X-eigenstates between each pair of operators, simplifying the resulting expression using

$$\left\langle x'\right|\, e^{-\delta P^2/2m}\,|x\rangle \propto e^{\frac{m}{2}\delta((x'-x)/\delta)^2}. \tag{2.10}$$

and identifying the ratio $(x'-x)/\delta$ with the velocity along a classical path, results in an expression which can be expressed as an integral of a classical action over classical trajectories.

Common methods for evaluating the integral over paths are: perturbation theory; making a stationary phase approximation; latticizing the continuum action and attempting to evaluate the resulting integral by Monte-Carlo methods. A problem with latticizing the continuum path-integral is that one must take small lattice-spacing to make contact with continuum physics which, of course, increases the complexity of the calculation and decreases the rate of convergence of the Monte-Carlo procedure. A goal of this paper is to develop improved actions which permit high accuracy computations for finite values of δ.

2.2 Beyond The Feynman Approximation

In what follows I refer to the replacement of $e^{-\delta H}$ by a product of exponentials as the Feynman approximation, even though this goes under a variety of other names. Since this approximation is the crucial first step in the derivation of the path-integral it is natural to see if it can be improved. I will discuss this question, derive several improved approximations and show how to apply them to various problems. While real understanding of the simplifications which arise requires studying this question on a Hamiltonian by Hamiltonian basis, there are some general remarks which should be made.

For a Hamiltonian of the form $H = A + B$, the Feynman approximation is commonly understood to be,

$$e^{-\delta(A+B)} = e^{-\delta A}\, e^{-\delta B}\, e^{\mathcal{O}(\delta^2)} \tag{2.11}$$

where $\mathcal{O}(\delta^2)$ is given by

$$\mathcal{O}(\delta^2) = -\frac{1}{2}\delta^2[A,B] - \delta^3\left(\frac{1}{6}[A,[A,B]] + \frac{1}{3}[B,[A,B]]\right) + \mathcal{O}(\delta^4) \tag{2.12}$$

Although this expression shows that $e^{\mathcal{O}(\delta^2)}$ can be replaced by unity in the limit $\delta \to 0$, it is not the optimal formula to use in order to minimize the errors for finite δ. One simple way to improve upon this formula is to adopt the more symmetric form

$$e^{-\delta(A+B)} = e^{-\delta A/2}\, e^{-\delta B/2}\, e^{C_3(\delta)}\, e^{-\delta B/2}\, e^{-\delta A/2} \tag{2.13}$$

where $C_3(\delta)$ has the expansion

$$\begin{aligned} C_3(\delta) = &-\delta^3\left(\frac{1}{12}[B,[A,B]] + \frac{1}{24}[A,[A,B]]\right) \\ &-\delta^5\left(\frac{1}{480}[B,[A,[A,[A,B]]]] - \frac{1}{480}[[A,B],[A,[A,B]]]\right. \\ &\quad + \frac{1}{320}[B,[B,[A,[A,B]]]] - \frac{1}{240}[[A,B],[B,[A,B]]] \\ &\quad \left. + \frac{1}{1920}[A,[A,[A,[A,B]]]] + \frac{1}{480}[B,[B,[B,[A,B]]]]\right) \\ &+ \mathcal{O}(\delta^7) \end{aligned} \tag{2.14}$$

This form has several advantages: first, even powers of δ vanish and second, the coefficients of the terms which remain are considerably smaller. The derivation of the formula used to compute this generic form is given in Appendix A but even a cursory comparison of Eq. (2.14) and Eq. (2.12) reveals why symmetric approximations contain no even powers of δ. The argument goes as follows: on general grounds the product $e^{\delta B/2}\, e^{\delta A/2} e^{-\delta(A+B)}\, e^{\delta A/2}\, e^{\delta B/2}$ can be written as $e^{D(\delta)}$, where $D(\delta)$ can be expanded as a sum of commutators of A and B. Since the logarithm of $e^{D(\delta)}$ must be a hermitian operator and since even powers of δ multiply odd numbers of commutators, which are anti-hermitian operators, the coefficients of even powers of δ must vanish.

3. Quantum Systems With One Degree of Freedom

3.1 The Harmonic Oscillator

The harmonic oscillator plays a central role in quantum mechanics and it is important to be sure that a new approximation technique works for this problem. This section compares the Feynman approximation for the harmonic oscillator to the higher-order approximations suggested by Eq. (2.13) and Eq. (2.14).

To simplify notation I will not write the Hamiltonian for the harmonic oscillator as

$$H = \frac{1}{2m} P^2 + \frac{m\omega^2}{2} X^2 \tag{3.1}$$

but will instead use the dimensionless operators

$$\begin{aligned} P' &= \frac{P}{\sqrt{m\omega}} \\ X' &= \sqrt{m\omega}\, X \\ H' &= H/m \end{aligned} \tag{3.2}$$

In other words, I will study the Hamiltonian

$$H = \frac{1}{2}P^2 + \frac{1}{2}X^2 \tag{3.3}$$

3.1.1 Three Approximations

The Feynman approximation to the harmonic oscillator Hamiltonian is

$$e^{-\delta H} \approx e^{-\frac{1}{2}\delta P^2} e^{-\frac{1}{2}\delta X^2} \tag{3.4}$$

and the lowest-order symmetric approximation, obtained by setting $C_3(\delta)$ to zero in Eq.(2.13), is

$$e^{-\delta H} \approx e^{-\frac{1}{4}\delta P^2}\, e^{-\frac{1}{2}\delta X^2}\, e^{-\frac{1}{4}\delta P^2} \tag{3.5}$$

Although the lowest-order symmetric approximation is an improvement upon the Feynman approximation, it would be nice to do better. This can be accomplished

using a variant of the lowest-order symmetric approximation, also discussed in the Appendix, which holds for an exponential of the sum of three operators; namely,

$$e^{-\delta(A+B+C)} = e^{-\delta A/2}\, e^{-\delta B/2}\, e^{-\delta C/2}\, e^{C_3'(\delta)}\, e^{-\delta C/2}\, e^{-\delta B/2}\, e^{-\delta A/2} \tag{3.6}$$

As before,

$$C_3'(\delta) = \sum_{n=1}^{\infty} \delta^{2n+1}\, \mathcal{O}'(2n+1)$$

and the first non-vanishing term in $C_3'(\delta)$ is given by

$$\begin{aligned} C_3'(\delta) = -\delta^3 \Big(& \frac{1}{24}[A,[A,B]] + \frac{1}{24}[A,[A,C]] + \frac{1}{12}[B,[A,B]] \\ & + \frac{1}{12}[B,[A,C]] + \frac{1}{24}[B,[B,C]] + \frac{1}{12}[C,[A,B]] \\ & + \frac{1}{12}[C,[A,C]] + \frac{1}{12}[C,[B,C]] \Big) \end{aligned}$$

The trick is to apply this identity to the operator $e^{C_3(\delta)}$ and rewrite it as

$$e^{C_3(\delta)} = e^{\delta B' P^2/2}\, e^{\delta A' X^2/2}\, e^{C_9(\delta)}\, e^{\delta A' X^2/2}\, e^{\delta B' P^2/2} \tag{3.7}$$

for an appropriate choice of $\delta A' X^2$ and $\delta B' P^2$. The choice of $\delta A' X^2$ and $\delta B' P^2$ is determined from the form of $C_3(\delta)$ by the requirement that the correction terms begin in order δ^9. Since in this case $C_3(\delta)$ has the form

$$\begin{aligned} C_3(\delta) \approx & -\frac{1}{12}\left(\delta^3 + \frac{7\delta^5}{40} + \frac{17\delta^7}{560} + \ldots\right) X^2 \\ & -\frac{1}{8}\left(-\frac{\delta^3}{3} + \frac{\delta^5}{30} + \frac{\delta^7}{280} - \ldots\right) P^2 \end{aligned} \tag{3.8}$$

the choice which accomplishes this is

$$\begin{aligned} \delta A' X^2 &= -\frac{1}{12}\left(\delta^3 + \frac{7\delta^5}{40} + \frac{17\delta^7}{560}\right) X^2 \\ \delta B' P^2 &= -\frac{1}{8}\left(-\frac{\delta^3}{3} + \frac{\delta^5}{30} + \frac{\delta^7}{280}\right) P^2 \end{aligned} \tag{3.9}$$

Because $\delta A'$ and $\delta B'$ contain all the terms which multiply either X^2 or P^2 up to

order δ^9, $C_3(\delta)$ can be written as

$$C_3(\delta) = \delta\, A' X^2 + \delta\, B' P^2 + \delta\, R'$$

where $\delta\, R'$ contains all terms of order δ^9 and higher. Applying the formula for an exponential of a sum of three operators to this expression produces

$$e^{-\delta H} \approx e^{-\frac{1}{4}\delta P^2}\, e^{-\frac{1}{4}\delta X^2}\, e^{\delta\, B' P^2/2}\, e^{\delta\, A' X^2/2}\, e^{C_9(\delta)}\, e^{\delta\, A' X^2/2}\, e^{\delta\, B' P^2/2}\, e^{-\frac{1}{4}\delta X^2}\, e^{-\frac{1}{4}\delta P^2} \tag{3.10}$$

It follows from the fact that $C_9(\delta)$ is a sum of multiple commutators of $\delta\, A'$, $\delta\, B'$ and $\delta\, R'$ that $C_9(\delta)$ starts in order δ^9. Appendix A contains explicit higher-order formulas for these identities as well as a discussion of the derivation of the lowest-order symmetric approximations for sums of operators.

The compactness of the expression for $C_3\,(\delta)$ is due to the fact that the operators P^2, X^2 and $S = iXP + 1/2$ form a closed algebra, with the commutation relations

$$\begin{aligned} \left[X^2, P^2\right] &= 4S \\ \left[P^2, S\right] &= 2P^2 \\ \left[S, X^2\right] &= 2X^2 \end{aligned} \tag{3.11}$$

It is clear from these relations that the commutators which appear in the general formula can all be replaced by P^2, X^2 and S; actually, since only odd powers of δ appear in the symmetric approximation there are no terms involving S. While this extreme simplification happens only for the harmonic oscillator, simplifications occur for other problems as well.

3.1.2 Comparing The Accuracy Of Different Approximations

It is convenient to compare the various operator approximations to $e^{-\delta H}$ by comparing their expectation values in a state of the form

$$\begin{aligned} |\gamma\rangle &= \left(\frac{\gamma}{\pi}\right)^{1/4} \int dx\, e^{-\gamma x^2/2}\, |x\rangle \\ &= (1/\pi\gamma)^{1/4} \int dp\, e^{-p^2/2\gamma}\, |p\rangle \end{aligned} \tag{3.12}$$

where $|x\rangle$ and $|p\rangle$ are eigenvectors of X and P and γ is an arbitrary, real, positive parameter. Since the state $|\gamma = 1\rangle$ is the lowest eigenstate of the true Hamiltonian, any failure to reproduce the correct answer, $Z_{\text{exact}}(\delta) = e^{-\delta/2}$, is due to a breakdown of the approximation; so comparing these expectation values provides

a measure of the relative accuracy of the operator approximations. Comparison of expectation values for $\gamma \neq 1$ checks both the validity of the operator approximations for higher states and the rate at which the contributions from higher states are suppressed as one goes to larger δ.

Carrying out the gaussian integrations for the Feynman approximation leads to

$$\langle\gamma|\, e^{-\delta p^2/2}\, e^{-\delta x^2/2}\, |\gamma\rangle = \frac{2\sqrt{2\gamma}}{\sqrt{4\gamma + 2\delta + \delta^2\gamma}\,\sqrt{2+\delta\gamma}} \tag{3.13}$$

Specializing to $\gamma = 1$ we obtain

$$\langle 1|\, e^{-\delta p^2/2}\, e^{-\delta x^2/2}\, |1\rangle = \frac{2\sqrt{2}}{\sqrt{4 + 2\delta + \delta^2}\,\sqrt{2\delta}} \tag{3.14}$$

The gaussian integrations for the more complicated case of the symmetric approximations can be done by means of the recursion relation

$$\langle\gamma|\, e^{-A_1 p^2}\, e^{-B_1 x^2}\, O\, e^{-B_1 x^2}\, e^{-A_1 p^2}\, |\gamma\rangle = N(\gamma, A_1, B_1)\, \langle\gamma'|\, O\, |\gamma'\rangle \tag{3.15}$$

where

$$\begin{aligned} \gamma'(\gamma, A, B) &= \frac{\gamma + 2B + 4BA\gamma}{1 + 2A\gamma} \\ N(\gamma, A, B) &= \left(\frac{\gamma}{\gamma'}\right)^{1/2} \frac{1}{1 + 2A\gamma} \end{aligned} \tag{3.16}$$

Applying Eq. (3.16) to the higher order symmetric approximation yields

$$Z_\gamma^{sa} = \frac{1}{\sqrt{1 + \frac{\delta^2}{2!} + \frac{\delta^4}{4!} + \frac{\delta^6}{6!} + \frac{1}{2}\,(1/\gamma + \gamma)\left[\delta + \frac{\delta^3}{3!} + \frac{\delta^5}{5!} + \frac{\delta^7}{7!}\right] + \ldots}} \tag{3.17}$$

which for $\gamma = 1$ becomes

$$Z_1^{sa} = \frac{1}{\sqrt{1 + \delta + \frac{\delta^2}{2!} + \frac{\delta^3}{3!} + \frac{\delta^4}{4!} + \frac{\delta^5}{5!} + \ldots + \frac{17\,\delta^{25}}{539492352000}}} \tag{3.18}$$

This shows that when $\gamma = 1$ the function Z^{sa} is one over the square root of a function whose Taylor series agrees with that for e^δ up to terms of order δ^9.

As $Z(\delta)$ dies exponentially for $\gamma = 1$, it is hard to see the discrepancies between different approximations on a linear plot; it is better to plot $\mathcal{E}(\delta)$, since it should take the constant value of $1/2$. Fig. 1 compares plots of $\mathcal{E}(\delta)$ for $0 \leq \delta \leq 1.5$ for the case of the Feynman approximation, first symmetric approximation ($C_3 = 0$) and the next higher order symmetric approximation. It is immediately apparent from the plot that even the lowest order symmetric approximation improves upon the naive Feynman approximation, however the way in which the next order symmetric approximation hugs the exact answer out to $\delta \approx 1$ is quite remarkable. The plot shown in Fig. 2 shows the same quantities for the case $\gamma = 2$ to show what happens starting from a state that has a 50% admixture of higher states. Once again, the lowest order symmetric approximation does better than the naive Feynman approximation, but the next order symmetric approximation follows the exact answer all the way to $\delta \approx 1$. This shows that minimizing the formula for $\mathcal{E}(\delta)$ with respect to γ for any value of $\delta < 1$ will, to high accuracy, produce the answer $\gamma = 1$.

3.1.3 Consequences

It is interesting to note that the structure of the higher order symmetric approximations provides another way of seeing the harmonic oscillator is a solvable problem. Because commuatators of X^2 , P^2 and $S = iXP + 1/2$ close among themselves, it is possible to approximate $e^{-\delta H}$ as an alternating, symmetric product of exponentials of P^2 and X^2 to arbitrary accuracy. The exact ground-state energy can be found by recursively evaluating the expectation value of the resulting product of operators in a Gaussian wavefunction. While this solution is not an improvement upon more direct methods it is interesting to see the way in which things work.

A more relevant question is "Does the higher order symmetric approximation lead to a path-integral formalism which, for given accuracy, requires fewer time slices than one based upon the Feynman approximation?". To answer this question compare the columns in Table 1 listing the percentage errors for the Feynman approximation and for the higher order symmetric approximation. It is clear that to achieve a percentage accuracy of .000049 in the Feynman approximation it is necessary to work at $\delta \approx .01$ as opposed to $\delta \approx .80$ for the higher-order symmetric approximation. In other words, to get this percentage accuracy using the Feynman approximation requires evaluating the expectation value of $C(\delta)^{80}$, rather than evaluating Eq. (3.10) with $C_9(\delta)$ set to unity. The evaluation of

$$\left\langle x \left| C(\delta)^{80} \right| x' \right\rangle$$

requires inserting complete sets of states between every factor, in other words, doing a seventy-nine slice path-integral, On the other hand, doing the same for

Eq. (3.10) yields a three time-slice path-integral. Thus, the higher order symmetric approximation wins by about a factor of twenty-seven. If the goal is merely one-tenth of one percent accuracy then the higher order approximation wins by about a factor of twenty.

As long as a symmetric approximation of the form

$$C_{\rm symm}(\delta) = e^{-\frac{1}{4}\delta P^2}\, e^{-\frac{1}{4}\delta X^2}\, e^{A_3(\delta)P^2}\, e^{2B_3(\delta)X^2}\, e^{A_3(\delta)P^2}\, e^{-\frac{1}{4}\delta X^2}\, e^{-\frac{1}{4}\delta P^2}$$

is valid, matrix elements of

$$\langle\gamma|\, C_{\rm symm}(\delta/2)^2\, |\gamma\rangle$$

must be equal to corresponding matrix elements of

$$\langle\gamma|\, C_{\rm symm}(\delta)\, |\gamma\rangle$$

This provides a measure of the accuracy of the operator approximation, and makes it possible, in the absence of the exact solution, to determine the value of δ beyond which the higher-order symmetric approximation breaks down.

3.2 The Anharmonic Oscillator

The anharmonic oscillator is defined by the Hamiltonian

$$H = \frac{1}{2}P^2 + \lambda X^4 \tag{3.19}$$

This problem is of interest for two reasons: first, because the problem is not exactly solvable—even the lowest order symmetric approximation exhibits structure which does not show up in the case of the simple harmonic oscillator; second, because the the lowest order symmetric approximation reveals both the reason for the lack of convergence of Padé approximants to the naive t-expansion and how the symmetric approximation avoids this problem.

As in the case of the simple harmonic oscillator the lowest order symmetric approximation is defined by the formula

$$e^{-\delta H} = e^{-\frac{1}{4}\delta P^2}\, e^{-\frac{1}{2}\delta\lambda X^4}\, e^{C_3(\delta)}\, e^{-\frac{1}{2}\delta\lambda X^4}\, e^{-\frac{1}{4}\delta P^2} \tag{3.20}$$

In this case, however, the term $C_3(\delta)$ is more complicated i.e.,

$$\begin{aligned} C_3(\delta) = &- \frac{\delta^3\lambda}{4} - \frac{\delta^3\lambda}{3}\left(2S + S^2 - \frac{1}{2}X^2P^2 + 4\lambda X^6\right) \\ &- \frac{\delta^5\lambda}{5}\left(14\lambda^2 X^8 + 4\lambda X^2 S + 6\lambda X^2 + \frac{1}{16}P^4 - \lambda X^4 P^2\right) \\ &+ \quad \delta^7 \ldots \end{aligned} \tag{3.21}$$

where, as before, $S = iXP$. This complexity makes it impossible to completely avoid expansions in δ when going beyond the approximation $e^{C_3(\delta)} = 1$, since exponentials of operators like X^2S or P^2X^2 cannot be evaluated in closed form. A minimal strategy for working with the higher-order approximations is to keep terms which just involve powers of X in the exponential and expand operators like $e^{i\delta X^4 P^2}$ or $e^{\delta X^2 S}$. For example, without any loss of accuracy rewrite $e^{C_3(\delta)}$ as

$$e^{C_3(\delta)} = e^{-\delta^3\lambda/4}\, e^{-F_1(\delta,\lambda,X)/2}\, e^{C_3'(\delta)}\, e^{-F_1(\delta,\lambda,X)/2} \tag{3.22}$$

where

$$\begin{aligned} F_1(\delta,\lambda,X) &= \frac{4\delta^3\lambda^2}{3}X^6 + \frac{6\delta^5\lambda^2}{5}X^2 + \frac{14\delta^5\lambda^3}{5}X^8 \\ C_3'(\delta) &= -\frac{\delta^3\lambda}{3}\left(2S + S^2 - \frac{1}{2}X^2P^2\right) \\ &\quad - \frac{\delta^5\lambda}{5}\left(4\lambda X^2 S + \frac{1}{16}P^4 - \lambda X^4 P^2\right) \\ &\quad + \quad \delta^7 \ldots \end{aligned} \tag{3.23}$$

and expand $e^{C_3'(\delta)}$ as a power series in δ. In this way the problem of computing $Z(\delta)$ is reduced to computing expectation values of the form

$$Z(\delta) = \sum_{n=0}^{\infty} \langle \Psi_{\text{eff}} | \, O_n \, | \Psi_{\text{eff}} \rangle \tag{3.24}$$

where

$$|\Psi_{\text{eff}}\rangle = \left(\frac{\gamma}{\pi}\right)^{1/4} \int dx\, e^{-\gamma x^2/(2+\delta\gamma) - F_1(\delta,\lambda,x)} \, |x\rangle \tag{3.25}$$

and the operators O_n are polynomials in X and P.

While expanding $e^{C_3'(\delta)}$ in powers of δ reduces the range for which the symmetric approximation is valid, since only part of the expression is expanded in δ, the

resulting formula should be more accurate than that provided by the naive t-expansion. As I will argue in the next section, Padé approximants based upon this modified series should be much more convergent than those done for the naive t-expansion.

3.2.1 Comparison to the Naive t-expansion

To apply the naive t-expansion to the case of the anharmonic oscillator expand

$$\langle\gamma|\, e^{-\delta(P^2/2+\lambda X^4)}\,|\gamma\rangle \tag{3.26}$$

as a power-series in δ, compute the various operator expectation values and then reconstruct $Z(\delta)$ or its logarithmic derivative by means of Padé approximants. A simple argument indicates that even though every term in the expansion is finite for $\gamma > 0$, Padé approximants to this series will have trouble converging. To see this ignore the P^2 term in the Hamiltonian and note that the expectation value

$$Z(\gamma,\delta) = \langle\gamma|\, e^{-\delta\lambda X^4)}\,|\gamma\rangle \tag{3.27}$$

diverges for negative λ, independently of the value chosen for γ. The lack of convergence of the Padé approximants reflects the fact that they are unsuccessfully trying to reconstruct singular behavior at $\lambda = 0$. In contrast to the t-expansion, both the Feynman and symmetric approximations keep the term λX^4 in the exponent. This means that without ignoring the P^2 term they exhibit singular behavior for $\lambda < 0$ and $\gamma > 0$. Of course, neither approximation directly reveals the structure of the true singularity at $\lambda = 0$, which is that the function Z is a function of $\delta\lambda^{1/3}$. A simple rescaling argument shows why this is the case. Consider the canonical transformation

$$\begin{aligned} P' &= \beta P \\ X' &= \beta^{-1} X \end{aligned} \tag{3.28}$$

and substitute this definition in Eq. (3.19) to obtain

$$H = \frac{\beta^2}{2} P'^2 + \frac{\lambda}{\beta^4} X^4 \tag{3.29}$$

Setting $\beta = \lambda^{1/6}$ gives

$$H = \lambda^{1/3}\left[\frac{1}{2}P'^2 + X^4\right] \tag{3.30}$$

where the only λ dependence is the overall multiplicative factor of $\lambda^{1/3}$, which shows that $Z(\delta)$ and $\mathcal{E}(\delta)$ are actually functions of $\delta\lambda^{1/3}$.

An interesting feature of both the naive t-expansion and the higher order symmetric approximation is that even without this rescaling, minimizing

$$\mathcal{E}(\gamma,\delta) = -\frac{d}{d\delta}\ln(Z(\gamma,\delta))$$

with respect to the variational parameter γ for $\delta \ll 1$ immediately reveals the fact that the energy is a function of $\delta\lambda^{1/3}$. In fact, if we generalize the problem to include a mass term, i.e.

$$H = \frac{1}{2}P^2 + \frac{\omega^2}{2}X^2 + \lambda X^4 \tag{3.31}$$

and minimize $\mathcal{E}(\gamma,\omega,\lambda,\delta=0)$ with respect to γ we obtain

$$\frac{1}{4} - \frac{\omega^2}{4\gamma^2} - \frac{12\lambda}{4\gamma^3} = 0 \tag{3.32}$$

which shows that $\mathcal{E}(\delta)$ is a function of $\delta\lambda^{1/3}$ for $\omega/\lambda^{1/3} < 1$. Deriving this result from a naive perturbative expansion is not easy [2].

3.2.2 Techniques For Obtaining Better Answers

While I have emphasized obtaining accurate operator approximations to $e^{-\delta H}$, as in the case of the simple harmonic oscillator, computing the ground-state energy to high accuracy also requires a good trial wave-function. The introduction of the variational parameter, γ, is a step in this direction but there are other tricks one can use. One such trick is to diagonalize a truncated version of the operator $e^{-\delta H}$.

3.2.2.1 A Finite Matrix Approximation

As always, the general problem is to maximize the expectation value

$$\langle\psi_{\text{trial}}|\, e^{-\delta H}\, |\psi_{\text{trial}}\rangle \tag{3.33}$$

In the preceding chapters $|\psi_{\text{trial}}\rangle$ was chosen to make the computation of Eq. (3.33) as simple as possible; however, to obtain higher accuracy one can consider a nor-

malized trial state of the form

$$|\psi_{\text{trial}}\rangle = \sum_{j=1}^{N} \alpha_j |\psi_j\rangle \tag{3.34}$$

where the $|\psi_j\rangle$'s are linearly independent states and the α_j's are arbitrary variational parameters. The expectation value of $e^{-\delta H}$ in this state is

$$\sum_{i,j=1}^{N} \alpha_i^* \alpha_j \langle\psi_i| e^{-\delta H} |\psi_j\rangle \tag{3.35}$$

Maximizing Eq.(3.35), subject to the constraint $\langle\psi_{\text{trial}}|\psi_{\text{trial}}\rangle = 1$, implies

$$\sum_{j=1}^{N} \langle\psi_i| e^{-\delta H} |\psi_j\rangle \alpha_j = \mu \sum_{j=1}^{N} \langle\psi_i|\psi_j\rangle \alpha_j \tag{3.36}$$

which says that the vector whose components are α_i is an eigenvector of the $N \times N$ matrix $\langle\psi_i| e^{-\delta H} |\psi_j\rangle$ relative to the metric $M_{ij} = \langle\psi_i|\psi_j\rangle$. Building a variational state out of orthonormal states of the form

$$|n, \gamma\rangle \approx \mathrm{H}_n(\gamma x)\, e^{-\gamma x^2/2} \tag{3.37}$$

where $\mathrm{H}_n(x)$ is the n^{th} Hermite polynomial, $\delta \approx 1/2$ and $n = 0, 2, 4, 6, 8$ it is possible to numerically calculate the ground-state energy to an accuracy of a part in 10^8 for a wide range of couplings.

3.2.2.2 Using Coherent States

Though it is customary to construct trial-states out of orthonormal wavefunctions, it is neither necessary nor always desirable to do so. At times it is simpler to evaluate the necessary matrix elements using normalized, linearly independent, states which are not orthogonal to one another. For example, consider building a trial wavefunction from a sum of coherent states of the form

$$|\gamma, c\rangle = e^{-iPc} |\gamma\rangle = \left(\frac{\gamma}{\pi}\right)^{1/4} e^{-\gamma(x-c)^2/2} \tag{3.38}$$

In this case carrying out the variational calculation requires evaluating matrix

elements of the form

$$\langle \gamma, c' |\, e^{-\delta\left[\frac{1}{2}P^2+V(X)\right]}\, |\gamma, c\rangle = \langle \gamma |\, e^{iPc'}\, e^{-\delta\left[\frac{1}{2}P^2+V(X)\right]}\, e^{-iPc}\, |\gamma\rangle \tag{3.39}$$

where the state $|\gamma, c\rangle$ is defined to be a translation of the state $|\gamma\rangle$

$$|\gamma, c\rangle = e^{iPc}\, |\gamma\rangle$$

The virtue of shifted Gaussians is that computation of matrix elements of the form Eq. (3.39) is quite straightforward. One way to automate this procedure is to introduce annihilation and creation operators A and $A^\dagger$ such that

$$\begin{aligned} X &= \sqrt{\frac{1}{2\gamma}}(A + A^\dagger) \\ P &= -i\sqrt{\frac{\gamma}{2}}(A - A^\dagger) \end{aligned} \tag{3.40}$$

so that

$$A\, |\gamma\rangle = 0 \tag{3.41}$$

and

$$\left[A, A^\dagger\right] = 1 \tag{3.42}$$

With these definitions it is simple to show that

$$\begin{aligned} e^{(\alpha A+\beta A^\dagger)} &= e^{-\alpha\beta/2}\, e^{\beta A^\dagger}\, e^{\alpha A} \\ e^{iPc}\, X\, e^{-iPc} &= X + c \\ e^{\alpha A}\, X e^{-\alpha A} &= X + \frac{\alpha}{\sqrt{2\gamma}} \\ e^{\alpha A}\, P e^{-\alpha A} &= P + i\,\alpha\sqrt{\frac{\gamma}{2}} \end{aligned} \tag{3.43}$$

Using these formulae we see that the inner-product of two shifted Gaussians is

$$\begin{aligned} \langle \gamma, c' | \gamma, c\rangle &= \langle \gamma |\, e^{iP(c'-c)}\, |\gamma\rangle \\ &= e^{-\gamma(c'-c)^2/4}\, \langle \gamma |\, e^{-\sqrt{\gamma/2}A^\dagger}\, e^{\sqrt{\gamma/2}A}\, |\gamma\rangle \\ &= e^{-\gamma(c'-c)^2/4} \end{aligned} \tag{3.44}$$

and the matrix-element $\langle \gamma, c' |\, e^{-\delta H}\, |\gamma, c\rangle$ can, without approximation, be written

as

$$\langle \gamma, c' | \, e^{-\delta\left[\frac{1}{2}P^2+V(X)\right]} \, | \gamma, c \rangle = \langle \gamma | \, e^{iP(c'-c)} \, e^{-\delta\left[\frac{1}{2}P^2+V(X+c)\right]} \, | \gamma \rangle$$
$$= e^{-\gamma(c'-c)^2/4} \, \langle \gamma | \, e^{-\delta\left[\frac{1}{2}(P+i\gamma(c'-c)/2)^2+V(X+(c'+c)/2)\right]} \, | \gamma \rangle \tag{3.45}$$

Going further in the evaluation of this matrix-element requires using either the Feynman approximation or one of the symmetric approximations. Using the lowest-order symmetric approximation the calculation becomes

$$e^{-\frac{1}{4}\gamma(c'-c)^2} \, \langle \gamma | \, e^{-\frac{1}{4}\delta\left(P+\frac{i\gamma}{2}(c'-c)\right)^2} e^{-\delta V(X+\frac{1}{2}(c'+c))} \, e^{-\frac{1}{4}\delta\left(P+\frac{i\gamma}{2}(c'-c)\right)^2} \, | \gamma \rangle \tag{3.46}$$

where I have set $e^{C_3(\delta)}$ to unity. In order to evaluate this expression it is convenient to insert a complete set of intermediate states on both ends of the expression and rewrite (3.46) as

$$e^{-\frac{1}{4}\gamma(c'-c)^2} \int \frac{dp_1}{2\pi} \int \frac{dp_2}{2\pi} \int dx$$
$$\langle \gamma | \, e^{-\frac{1}{4}\delta\left(P+\frac{i\gamma}{2}(c'-c)\right)^2} \, | p_1 \rangle \, \langle p_1 | x \rangle \, e^{-\delta V(x+\frac{1}{2}(c'+c))} \, \langle x | p_2 \rangle \, \langle p_2 | \, e^{-\frac{1}{4}\delta\left(P+\frac{i\gamma}{2}(c'-c)\right)^2} \, | \gamma \rangle \tag{3.47}$$

Using the explicit form for $|\gamma\rangle$ as a function of p and doing a bit of algebra reduces this to an expression of the form

$$\frac{\sqrt{\gamma}}{\pi^{3/2}(2+\delta\gamma)} \, e^{-\gamma(c'-c)^2/(4+2\delta\gamma)} \int dx \, e^{-\delta V(x+\frac{1}{2}(c'+c))-2\gamma x^2/(2+\delta\gamma)} \tag{3.48}$$

which for narrow packets and small δ is, up to a normalization factor, the result which would be obtained from the usual derivation of the path-integral.

3.2.2.3 Connecting to the Stationary Phase Approximation

If one now decides to use a fixed number of shifted Gaussians, $|\gamma, c_i\rangle, i = 1 \ldots N$, to construct a trial state, one is left with the problem of determining the c_i's. A brute force method for determining them is to solve the relative eigenvalue problem and minimize the energy as a function of γ and c_i. Although this is guaranteed to produce the best results it can be difficult to minimize a function of several variables. An approach which cuts down on the number of variables which have to be varied, is to choose the c_i's to be multiples of a single parameter, c, i.e. $c_n = cn$. This approach can be very useful when dealing with problems like the

simple anharmonic oscillator, however it is not the best way to proceed if $V(x)$ is a function which has multiple minima, for example

$$V(x) = \lambda (x^2 - f^2)^2 \tag{3.49}$$

In such a case it is better to choose some of the states to lie at the classical minima and then do a calculation to determine the best states to add to this set in order to minimize the expectation value of the Hamiltonian. For the preceding example begin by calculating the expectation value $\langle \gamma, c | \, e^{-\delta H} \, | \gamma, c \rangle$ for a single coherent state and maximize this expectation value as a function of γ and c (that is minimize the energy). In the limit of large γ and small δ the c-dependent part of this expectation value is

$$\langle \gamma, c | \, e^{-\delta H} \, | \gamma, c \rangle \approx e^{-\delta \lambda (c^2 - f^2)^2} \tag{3.50}$$

Maximizing this with respect to c gives the two solutions, $|\gamma, \pm f\rangle$. Since both states yield the same value for the energy, the Rayleigh-Ritz procedure implies that one should diagonalize the 2×2 matrix

$$\begin{pmatrix} \langle \gamma, +f | \, e^{-\delta H} \, | \gamma, +f \rangle & \langle \gamma, +f | \, e^{-\delta H} \, | \gamma, -f \rangle \\ \langle \gamma, -f | \, e^{-\delta H} \, | \gamma, +f \rangle & \langle \gamma, -f | \, e^{-\delta H} \, | \gamma, -f \rangle \end{pmatrix} \tag{3.51}$$

which, using Eq.(3.48), is proportional to

$$\begin{pmatrix} 1 & e^{-\frac{\gamma}{2(2+\delta\gamma)}(2f)^2} \\ e^{-\frac{\gamma}{2(2+\delta\gamma)}(2f)^2} & 1 \end{pmatrix} \tag{3.52}$$

If γ is large enough that the states $|\gamma, \pm f\rangle$ are nearly orthogonal, simply diagonalizing this matrix produces reasonable results. Such a calculation would yield two states which are slightly split in energy; this is the correct qualitative behavior. If the separation of the two minima is large relative to the natural width of the packets, as determined by extremizing the single-state expectation value of $\langle \gamma, f | \, e^{-tH} \, | \gamma, f \rangle$ with respect to γ, this calculation seriously underestimates the true splitting because in the region between the two minima the exact wave-function does not fall off as a gaussian but as an exponential. To reproduce this behavior and obtain the correct splitting it is necessary to increase the number of states used in the trial wave-function by adding states $|\gamma, c_i\rangle$ whose centers, c_i, lie between the values $\pm f$. Deciding, a priori, to choose N additional states of this type, it only remains to determine how to choose the N c_i's so as to obtain

maximal mixing and therefore the best estimate of the true ground-state energy. The most accurate way to do this is to diagonalize the $(N+2)\times(N+2)$ matrix and minimize its lowest eigenvalue with respect to γ and the c_i's. Unfortunately, this is a formidable problem and it seems that adopting simpler but a non-optimal approach would seem to be in order. A possible procedure is to maximize the product

$$\langle \gamma, -f | e^{-\delta H} | \gamma, c_1 \rangle \ldots \langle \gamma, c_j | e^{-\delta H} | \gamma, c_{j+1} \rangle \ldots \langle \gamma, c_N | e^{-\delta H} | \gamma, f \rangle \tag{3.53}$$

which will provide a set of states which provide the best interpolation between the states $|\gamma, \pm f\rangle$. Using Eq. (3.47) and taking the limit of large γ, $\delta\gamma$ and small δ, this becomes proportional to

$$e^{-\delta \sum_j \left[\frac{1}{2}((c_{j+1}-c_j)/\delta)^2 + V(\frac{1}{2}(c_{j+1}+c_j))\right]} \tag{3.54}$$

In this limit, varying with respect to the c_j's leads to a discretized form of the usual stationary phase approximation for the Euclidean path-integral but significant corrections to the familiar formula arise even at the level of the lowest order symmetric approximation and for moderately small values of δ and γ. Of course, for finite γ it is necessary to correctly include the effects due to the non-orthogonality of the states when calculating the ground-state energy.

Eq. (3.54) implies that the conventional Euclidean stationary phase approximation is related to a simple variational calculation for the best set of states to use in a Rayleigh-Ritz calculation of the ground-state energy. Clearly, one way to improve upon these is to use the lowest symmetric approximation to determine the c_j's and then use matrix elements, computed in a higher order symmetric approximation, to set-up the Rayleigh-Ritz calculation. This has the advantage of producing fairly simple equations for the c_j's and still systematically incorporating higher order terms in δ when computing the ground-state energy.

4. Lattice Spin Systems: The Ising Model

Although discussing application of these techniques to other quantum mechanical systems would be interesting, it is more instructive to apply them to more complicated systems. This chapter discusses the application of variants of higher-order symmetric approximations to the one-dimensional quantum Ising model in a transverse magnetic field. Note, this model is equivalent to the two-dimensional Ising model studied in statistical mechanics and like its counterpart the 1+1–dimensional quantum Ising model is exactly solvable. This, of course, makes it a good test-bed for trying out approximation schemes.

The Hamiltonian of the one-dimensional Ising model is

$$H = -\sum_j [\sigma_z(j) + \lambda \sigma_x(j)\sigma_x(j+1)\,] \tag{4.1}$$

The exact solution to this model exhibits a second-order phase transition at $\lambda = 1$. For $\lambda < 1$ the ground-state of the system is unique and the order parameter, $\langle \sigma_x(j) \rangle = 0$. When $\lambda > 1$ the system has a twofold degenerate ground-state corresponding to the non-vanishing values of the order parameter,

$$\left\langle \sum \sigma_x(j) \right\rangle = \pm(1 - 1/\lambda^2)^{1/8}.$$

To intuitively understand this result consider the limiting cases, $\lambda = 0$ and $\lambda = \infty$. For $\lambda = 0$ the ground-state must be a simultaneous eigenstate of all of the operators $\sigma_z(j)$. This defines a unique state ψ, namely $|\psi\rangle = \prod_j |\uparrow\rangle_j$, where $|\uparrow\rangle_j$ is the single-site eigenstate of $\sigma_z(j)$ with eigenvalue $+1$. On the other hand, in the limit of large λ this state must be a simultaneous eigenstate of the operators $\sigma_x(j)\,\sigma_x(j+1)$ with eigenvalue $+1$. There are two possible states which satisfy these conditions

$$|\psi_R\rangle = \prod_j |{\rightarrow}\rangle_j \quad ; \quad |\psi_L\rangle = \prod |{\leftarrow}\rangle_j \tag{4.2}$$

where $|{\rightarrow}_j\rangle$ and $|{\leftarrow}_j\rangle$ are the single-site states such that

$$\sigma_x(j)\,|{\rightarrow}\rangle_j = |{\rightarrow}\rangle_j \quad ; \quad \sigma_x(j)\,|{\leftarrow}\rangle_j = -\,|{\leftarrow}\rangle_j \tag{4.3}$$

In the limit of infinite volume the states $|\psi_R\rangle$ and $|\psi_L\rangle$ do not mix to any finite order in perturbation theory and remain degenerate. Since simple perturbative arguments show that the degeneracy of the ground-state changes as λ goes from zero to infinity it follows that there must be a phase transition at some finite value of λ.

4.1 A Single-Site Symmetric Approximation

The most natural way to apply the lowest order symmetric approximation to the Ising model is to divide the Hamiltonian into two parts, each of whose matrix elements can be easily evaluated. One approach is to consider

$$\begin{aligned} A &= \sum_j \sigma_z(j) \\ B &= \sum_j \lambda\, \sigma_x(j)\sigma_x(j+1) \end{aligned} \tag{4.4}$$

so that $H = -A - B$ and rewrite

$$e^{-\delta(-A-B)} = e^{\delta A/2}\, e^{\delta B/2}\, e^{C_3(\delta)}\, e^{\delta B/2}\, e^{\delta A/2} \tag{4.5}$$

I will first discuss this approximation by setting $e^{C_3(\delta)}$ to unity, since this is what I did for the case of the harmonic oscillator; however, once I have set up the basic calculation I will return to a discussion of the structure of $C_3(\delta)$.

Once again choose the trial state to render the computation of the expectation value in Eq. (4.5) as simple as possible. Given that the operators in A all commute with one another, it is natural to use the $\lambda = 0$ ground-state; i.e.

$$Z(\delta) = \langle\uparrow \ldots \uparrow|\, e^{\frac{1}{2}\delta \sum_j \sigma_z(j)}\, e^{\delta\lambda \sum_j \sigma_x(j)\sigma_x(j+1)}\, e^{\frac{1}{2}\delta \sum_j \sigma_z(j)}\, |\uparrow \ldots \uparrow\rangle \tag{4.6}$$

Since this state is an eigenstate of all of the operators $\sigma_z(j)$ with eigenvalue $+1$ it follows immediately that

$$Z(\delta) = \left(e^{\delta}\right)^V \langle\uparrow \ldots \uparrow|\, e^{\delta\lambda \sum_j \sigma_x(j)\sigma_x(j+1)}\, |\uparrow \ldots \uparrow\rangle \tag{4.7}$$

Finally, applying the identity

$$e^{\delta\lambda\sigma_x(j)\,\sigma_x(j+1)} = \cosh(\delta\lambda) + \sinh(\delta\lambda)\, \sigma_x(j)\, \sigma_x(j+1) \tag{4.8}$$

we obtain

$$Z(\delta) = \left(e^{\delta}\cosh\delta\lambda\right)^V \langle\uparrow \ldots \uparrow|\, \prod_j \left(1 + \tanh(\delta\lambda)\, \sigma_x(j)\, \sigma_x(j+1)\right)\, |\uparrow \ldots \uparrow\rangle \tag{4.9}$$

To proceed, evaluate the expectation value of the product of operators appearing in Eq. (4.9). This is straightforward since the expectation value of $\sigma_x(j)$ vanishes

in the state $|\uparrow \ldots \uparrow\rangle$ and so the term 1 is the only term in the expansion of the product that doesn't vanish. Thus,

$$Z(\delta) = \left(e^{\delta} \cosh \delta\lambda\right)^{V} \tag{4.10}$$

and the energy density in this approximation is

$$\mathcal{E}(\delta) = -\frac{1}{V}\frac{d}{d\delta}\log\left(Z(\delta)\right) = -1 - \lambda \tanh\left(\delta\lambda\right) \tag{4.11}$$

Fig. 3 shows a plot of this approximation compared to the exact energy density for $\delta = .5, 1, 5$ for $0 < \lambda < 7$. Note, while Eq. (4.11) gives the exact answer for $\lambda = 0$ it undershoots the exact answer for $\delta = \infty$ or finite δ and large λ. To do better than this it is necessary to investigate the effect of including higher order terms in the expansion and/or choosing a different decomposition of the Hamiltonian. Actually, the next section will show that a more correct form of Eq. (4.11) is

$$\mathcal{E}(\delta) = -1 - \lambda \tanh\left(\delta\lambda/\sqrt{1+\lambda^2}\right) \tag{4.12}$$

This function behaves quite differently for large λ. Plots of this function are shown in Fig. 4.

4.1.1 Beyond The Lowest Order Approximation

One way to go beyond the lowest order approximation is to expand $e^{C_3(\delta)}$ as a product of exponentials of operators having coefficients which are polynomials in δ of order δ^7 and an exponential of a sum of terms whose coefficients begin in order δ^7. Application of the formula for $C_3(\delta)$ given in Appendix A to the definition of A and B given in Eq. (4.4) yields

$$\begin{aligned} C_3(\delta) = -\sum_j \Big(& \beta_z O_z(j) + \beta_{xx} O_{xx}(j) + \beta_{yy} O_{yy}(j) + \beta_{xzx} O_{xzx}(j) \\ & + \beta_{yzy} O_{yzy}(j) + \beta_{xzzx} O_{xzzx}(j) \Big) \end{aligned} \tag{4.13}$$

where

$$\begin{aligned}
\beta_z &= \left[\frac{2\lambda^2}{3}\,\delta^3 + \frac{4\lambda^2}{15}(2+\lambda^2)\,\delta^5 + \mathcal{O}(\delta^7)\right] \\
\beta_{xx} &= \left[-\frac{\lambda}{3}\,\delta^3 + \frac{\lambda}{15}(-1+8\lambda^2)\,\delta^5 + \mathcal{O}(\delta^7)\right] \\
\beta_{yy} &= \left[\frac{\lambda}{3}\,\delta^3 + \frac{\lambda}{15}(1-\lambda^2)\,\delta^5 + \mathcal{O}(\delta^7)\right] \\
\beta_{xzx} &= \left[\frac{2\lambda^2}{3}\,\delta^3 + \frac{2\lambda^2}{15}(3+2\lambda^2)\,\delta^5 + \mathcal{O}(\delta^7)\right] \\
\beta_{yzy} &= \left[\frac{2\lambda^2}{15}\,\delta^5 + \mathcal{O}(\delta^7)\right] \\
\beta_{xzzx} &= \left[-\frac{7\lambda^3}{15}\,\delta^5 + \mathcal{O}(\delta^7)\right]
\end{aligned} \tag{4.14}$$

and $O_{a_1\ldots a_n}(j)$ stands for the product

$$O_{a_1\ldots a_n}(j) = \sigma_{a_1}(j)\,\sigma_{a_2}(j+1)\ldots\sigma_{a_n}(j+n) \tag{4.15}$$

The same argument used for the harmonic and anharmonic oscillators says it is possible to rewrite $e^{C_3(\delta)}$ as

$$\begin{aligned}
e^{C_3(\delta)} =& e^{\frac{1}{2}\beta'_z \sum_j O_z(j)}\, e^{\frac{1}{2}\beta'_{xx} \sum_j O_{xx}(j)}\, e^{\frac{1}{2}\beta'_{yy} \sum_j O_{yy}(j)}\, e^{\frac{1}{2}\beta'_{xzx} \sum_j O_{xzx}(j)} \\
& e^{\frac{1}{2}\beta'_{yzy} \sum_j O_{yzy}(j)}\, e^{\frac{1}{2}\beta'_{xzzx} \sum_j O_{xzzx}(j)}\, e^{C_7(\delta)}\, e^{\frac{1}{2}\beta'_{xzzx} \sum_j O_{xzzx}(j)}\, e^{\frac{1}{2}\beta'_{yzy} \sum_j O_{yzy}(j)} \\
& e^{\frac{1}{2}\beta'_{xzx} \sum_j O_{xzx}(j)}\, e^{\frac{1}{2}\beta'_{yy} \sum_j O_{yy}(j)}\, e^{\frac{1}{2}\beta'_{xx} \sum_j O_{xx}(j)}
\end{aligned} \tag{4.16}$$

where $\beta'_{a_1\ldots a_n}$ are defined from the β's appearing in Eq. (4.14) by leaving off the terms of order δ^7 and higher. Setting $e^{C_3(\delta)} = 1\ Z(\delta)$ becomes

$$
\begin{aligned}
Z(\delta) = e^{V\delta} \cosh(\tfrac{1}{2}\delta\lambda)^{2V} & \\
& \left[\left(\cosh(\tfrac{1}{2}\beta'_z) \cosh(\tfrac{1}{2}\beta'_{xx}) \cosh(\tfrac{1}{2}\beta'_{yy}) \cosh(\tfrac{1}{2}\beta'_{xzx}) \cosh(\tfrac{1}{2}\beta'_{yzy}) \right)^2 \cosh(\beta'_{xzzx}) \right]^V \\
& \Big\langle \prod_{j_0} (1 + \tanh(\tfrac{1}{2}\delta\lambda) O_{xx}(j_0)) \prod_{j_1} (1 + \tanh(\tfrac{1}{2}\beta'_z) O_z(j_1)) \\
& \prod_{j_2} (1 + \tanh(\tfrac{1}{2}\beta'_{xx}) O_{xx}(j_2)) \prod_{j_3} (1 + \tanh(\tfrac{1}{2}\beta'_{yy}) O_{yy}(j_3)) \\
& \prod_{j_4} (1 + \tanh(\tfrac{1}{2}\beta'_{xzx}) O_{xzx}(j_4)) \prod_{j_5} (1 + \tanh(\tfrac{1}{2}\beta'_{yzy}) O_{yzy}(j_5)) \\
& \prod_{j_6} (1 + \tanh(\beta'_{xzzx}) O_{szzx}(j_6)) \prod_{j_7} (1 + \tanh(\tfrac{1}{2}\beta'_{yzy}) O_{yzy}(j_7)) \\
& \prod_{j_8} (1 + \tanh(\tfrac{1}{2}\beta'_{xzx}) O_{xzx}(j_8)) \prod_{j_9} (1 + \tanh(\tfrac{1}{2}\beta'_{yy}) O_{yy}(j_9)) \\
& \prod_{j_{10}} (1 + \tanh(\tfrac{1}{2}\beta'_{xx}) O_{xx}(j_{10})) \prod_{j_{11}} (1 + \tanh(\tfrac{1}{2}\beta'_z) O_z(j_{11})) \\
& \prod_{j_{12}} (1 + \tanh(\tfrac{1}{2}\delta\lambda) O_{xx}(j_{12})) \Big\rangle
\end{aligned}
\tag{4.17}
$$

where the operator expectation value is to be taken in the state $|\uparrow \ldots \uparrow\rangle$. Contrary to the lowest order approximation, the operator expectation value contains many non-vanishing terms and evaluation of these terms results in polynomials in the various $\beta_{a_1 \ldots a_n}$.

4.1.1.1 Computing The Energy Density

While Eq. (4.17) has resummed some of the δ and λ dependence of $Z(\delta)$, it does not produce a completely resummed formula for the energy density, $\mathcal{E}(\delta)$. To see the problems which remain and understand what must be done to avoid them consider the logarithmic derivative of $Z(\delta)$ in the approximation where the expectation value is taken to be unity.

$$
\begin{aligned}
\mathcal{E}(\delta) = & -1 - \lambda \tanh(\frac{\delta\lambda}{2}) \\
& - \left(\frac{4\lambda^2}{3}\delta^2 + \frac{20\lambda^2}{15}(2+\lambda^2)\delta^4 \right) \tanh\left(\frac{2\lambda^2}{3}\delta^2 + \frac{10\lambda^2}{15}(2+\lambda^2)\delta^4 \right) \\
& + \ldots
\end{aligned}
\tag{4.18}
$$

Eq. (4.18) is a mixture of polynomials in λ and δ times hyperbolic tangents of polynomials in the same variables. Although the hyperbolic tangent is a ratio of sums and differences of exponentials, the polynomials multiplying these functions make the evaluation of $\mathcal{E}(\delta)$ problematic for large values of δ and/or λ.

The problem with extending Eq. (4.18) to large λ has a simple and generic fix: rescale the Hamiltonian by a factor $1/\sqrt{1+\lambda^2}$. In other words, compute the ground-state energy for the Hamiltonian

$$H' = -\sum_j \left[\frac{1}{\sqrt{1+\lambda^2}}\sigma_z(j) + \frac{\lambda}{\sqrt{1+\lambda^2}}\sigma_x(j)\,\sigma_x(j+1)\right] \tag{4.19}$$

and then multiply the answer by $\sqrt{1+\lambda^2}$ to find the answer to the original problem. This method has the advantage that for both $\lambda = 0$ and $\lambda = \infty$ there is only one term in the Hamiltonian. Since making this change is equivalent to substituting $\delta = \delta/\sqrt{1+\lambda^2}$ in Eq.(4.18) we see that Eq.(4.18) becomes

$$\begin{aligned}\mathcal{E}(\delta) = &-1-\lambda\tanh\left(\frac{\delta\lambda}{\sqrt{1+\lambda^2}}\right)\\ &-\left(\frac{4\lambda^2}{3(1+\lambda^2)}\delta^2 + \frac{20\lambda^2(2+\lambda^2)}{15(1+\lambda^2)^2}\delta^4\right)\tanh\left(\frac{2\lambda^2}{3(1+\lambda^2)}\delta^2 + \frac{10\lambda^2(2+\lambda^2)}{15(1+\lambda^2)^2}\delta^4\right)\\ &+\ldots\end{aligned} \tag{4.20}$$

which is finite for all values of λ. Unfortunately, this trick does nothing to solve the problem of going to large δ. To go to large δ it is necessary to confront the problem of reconstructing power-series in δ with coefficients which are analytic functions of δ. While the answer might be as simple as treating the coefficients of the simple powers of δ as constants and using them to construct Padé approximants I see no clear justification for this procedure and the problem needs further study. Since the principal aim of this paper is to expose the general idea and explore the various possibilities which it suggests, I will not pursue this point further. Instead, I will discuss other ways to generate approximations which treat a larger part of the Hamiltonian exactly.

4.2 The Symmetric Approximation With Larger Blocks

Another approach to employing the symmetric approximation is to divide the Hamiltonian so that a larger part of the problem is treated exactly. For example, consider the following definition of the operators A and B:

$$\begin{aligned} A &= -\sum_p H(p) \\ &= -\sum_p \left(\sigma_z(2p) + \sigma_z(2p+1) + \lambda\, \sigma_x(2p)\, \sigma_x(2p+1) \right) \\ B &= -\sum_p V(p) \\ &= -\sum_p \lambda\, \sigma_x(2p+1)\, \sigma_x(2(p+1)) \end{aligned} \tag{4.21}$$

Since A is a sum of commuting the *block*–Hamiltonians, $H(p)$, to find the exact eigenstates of A just diagonalize each $H(p)$ separately.

As before begin by by setting $e^{C_3(\delta)}$, computed for this definition of A and B, set to unity. This means that in evaluating the matrix element of the operator product

$$e^{-\delta H} = e^{\frac{1}{2}\delta A}\, e^{\delta B}\, e^{\frac{1}{2}\delta A}$$

the eigenvalue of A factors out and the problem reduces to evaluating the expectation value of the exponential of the operators appearing in B. As I already noted, in order to find the lowest eigenstate of A it is only necessary to find the lowest eigenstate of any one of the $H(p)$'s, since each $H(p)$ has the same structure. This is trivial, however, because each $H(p)$ reduces to a two-site problem and so it suffices to discuss its matrix elements between the four states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$. Furthermore, since each $H(p)$ is invariant under the transformation which exchanges the operators on the sites $2p$ and $2p+1$ the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ and $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ mix separately. This means that diagonalizing $H(p)$ actually reduces to the problem of diagonalizing two independent 2×2 matrices. Since, in each subspace, $\sigma_z(2p)$ and $\sigma_z(2p+1)$ map these states into themselves and $\sigma_x(2p)\,\sigma_x(2p+1)$ maps one state into the other the matrices to be diagonalized are

$$\begin{array}{c} \\ |\uparrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{array} \begin{array}{c} \begin{array}{cc} |\uparrow\uparrow\rangle & |\downarrow\downarrow\rangle \end{array} \\ \begin{pmatrix} -2 & -\lambda \\ -\lambda & 2 \end{pmatrix} \end{array}$$

and

$$\begin{array}{c} \\ |\uparrow\downarrow\rangle \\ |\downarrow\uparrow\rangle \end{array} \begin{array}{c} \begin{array}{cc} |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle \end{array} \\ \begin{pmatrix} 0 & -\lambda \\ -\lambda & 0 \end{pmatrix} \end{array}$$

The eigenvalues of the first matrix are $\mp\sqrt{4+\lambda^2}$. and those of the second are $\mp\lambda$. This shows that the maximum eigenvalue of $e^{-\frac{1}{2}\delta A}$ is $e^{\delta\sqrt{4+\lambda^2}}$ and so, without further ado,

$$Z(\delta) = \left(e^{2\delta\sqrt{1+\lambda^2/4}}\cosh(\delta\lambda)\right)^{V/2} \left\langle \prod_p (1+\tanh(\delta\lambda)\,\sigma_x(2p+1)\,\sigma_x(2(p+1)) \right\rangle$$

Once again, since the ground-state of the block Hamiltonian is a linear combination of $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$, it follows that the expectation value of the product of operators is unity. Taking minus the logarithmic derivative of $Z(\delta)$ with respect to δ yields

$$\mathcal{E}(\delta) = -\sqrt{1+\lambda^2/4} - \frac{\lambda}{2}\tanh(\delta\lambda) \tag{4.22}$$

which goes to the exact answer both for $\lambda = 0$ and $\lambda = \infty$. A comparison of exact ground-state energy density and Eq.(4.22) is show in Fig.5.

This result is satisfactory if and only it is legitimate to ignore the term $e^{C_3(\delta)}$. If this term is taken into account then the energy density once again contains polynomials in λ and to get an expansion which is valid for large λ it is necessary to work with the rescaled Hamiltonian and multiply the final answer by $\sqrt{1+\lambda^2}$. This changes Eq. (4.22) to

$$\mathcal{E}(\delta) = -\sqrt{1+\lambda^2/4} - \frac{\lambda}{2}\tanh\left(\frac{\delta\lambda}{\sqrt{1+\lambda^2}}\right) \tag{4.23}$$

Unlike Eq. (4.22) , Eq. (4.23) only gives the exact energy density for large λ in the limit of $\delta \to \infty$; this, however, is what is to be expected.

4.2.1 Further Observations

The fact that $[A, B]$ contains only terms which join two blocks means that the higher commutators appearing in the expansion of $C_3(\delta)$ give rise to products of the form $O_{a_1\ldots a_n}(j)$ which cross a block boundary. Since there are fewer terms of this sort, this means that the effect of these terms on the energy density is reduced relative to what it would be for a higher-order symmetric approximation

based upon single-site blocks. The structure of these terms and the way they drop off in importance is made even more apparent by considering a decomposition based upon bigger blocks. For example, define A as a sum of commuting sub-Hamiltonians each of which contains all terms in H which involve operators which lie totally within a single block of length L; i.e.

$$\begin{aligned} A &= -\sum_p H(p) \\ &= -\sum_p \left(\sum_{r=0}^{L-1} \sigma_z(Lp+r) + \sum_{r=0}^{L-2} \lambda\, \sigma_x(Lp+r)\, \sigma_x(Lp+r+1) \right) \\ B &= -\sum_p V(p) \\ &= -\sum_p \lambda\, \sigma_x(L(p+1)-1)\, \sigma_x(L(p+1)) \end{aligned} \tag{4.24}$$

Following the approach used earlier in the discussion of the higher order terms, rewrite $e^{C_3(\delta)}$ as in Eq. (4.16), except now the various operators are concentrated near the boundaries of the block. So, for example, the term $e^{\frac{1}{2}\beta'_z \sum_j O_z(j)}$ becomes $e^{\frac{1}{2}\beta'_z \sum_p O_z((L+1)p-1)+O_z((L+1)p)}$. Since there are only two such operators for each block p, this simplifies to

$$\begin{aligned} \cosh(\tfrac{1}{2}\beta'_x)^{2V/L} \prod_p \Big(1 + \tanh(\tfrac{1}{2}\beta'_z O_z((L+1)\,p-1) \Big) \\ \Big(1 + \tanh(\tfrac{1}{2}\beta'_z O_z((L+1)\,p) \Big) \end{aligned} \tag{4.25}$$

Thus the contribution to the energy density of terms proportional to powers of $\cosh(\beta'_{\ldots})$ are multiplied by explicit powers of $1/L$ and contribute a smaller amount to the energy density. Of course, it is still necessary to evaluate the expectation value of the product of operators appearing in the expansion of $e^{C_3(\delta)}$ but the number non-trivial terms in this expansion are also greatly reduced from the case of the single-site blocks. Furthermore, the calculation of these terms for low orders of $\tanh(\delta \ldots)$ is quite simple due to the fact that

$$\Big\langle O_{a_1 \ldots a_n}(j_1) O_{b_1 \ldots b_m}(j_2) \Big\rangle \approx \Big\langle O_{a_1 \ldots a_n}(j_1) \Big\rangle \Big\langle O_{b_1 \ldots b_m}(j_2) \Big\rangle, \tag{4.26}$$

at least for $|j_1 - j_2| > m + n$.

While it would be interesting to pursue the structure of this series further I will leave that for another paper.

4.3 Effective Potential or Mean-Field Methods

Although a symmetric approximation built upon multi-site blocks allows one to compute the ground-state energy of the Ising model to high accuracy, extracting the location and properties of a phase transition from such a calculation will be difficult. In this section I show how incorporating "mean-field" (or "effective potential") ideas into the symmetric approximation scheme simplifies the task.

Both the single-site and two-site block calculations described in the preceding sections obscure the physics of the phase transition because they start from the lowest eigenstate of the operator A in order to simplify the computation. The expectation value of the order parameter, $\sigma_x(j)$, will always vanish in this state because it is invariant under the transformation which takes $\sigma_x(j)$ to $-\sigma_x(j)$. To avoid this incorrect result one must use a trial-state which allows for a non-vanishing value of $\sigma_x(j)$, which immediately suggests a variational approach to the problem of choosing the best trial state.

There are many ways to introduce a variational wave-function into this problem, I will limit myself to discussing one possibility. In this approach one first computes the ground-state energy density of a family of Hamiltonians which differ slightly from the Ising Hamiltonian and then converts the results into a one-parameter family of "bounds" on the ground-state energy density of the unmodified problem. One then minimizes these bounds with respect to the free parameter so as to produce the "best" bound on the true ground-state energy density.

Begin by considering the family of Hamiltonians, $H(J)$,

$$\begin{aligned} H(J) =& H_{\text{Ising}} + J \sum_j \sigma_x(j) \\ & - \sum_j \Big[\sigma_z(j) + J\,\sigma_x(j) + \lambda\,\sigma_x(j)\,\sigma_x(j+1) \Big] \end{aligned} \tag{4.27}$$

and attempt to compute the ground-state energy for each value of J using a symmetric approximation based upon the decomposition of $H(J)$

$$H(J) = A(J) + B \tag{4.28}$$

where

$$\begin{aligned} A(J) &= -\sum_j \left(\sigma_z(j) + J\sigma_x(j)\right) \\ B &= -\sum_j \lambda\sigma_x(j)\,\sigma_x(j+1) \end{aligned}$$

As in earlier calculations, the simplest use of the lowest order symmetric approxi-

mation rewrites $\left\langle e^{H(J)} \right\rangle$ as

$$\left\langle e^{-\frac{1}{2}\delta A(J)}\, e^{-\delta B}\, e^{-\frac{1}{2}\delta A(J)} \right\rangle \tag{4.29}$$

and evaluates the expectation value in the ground-state of $A(J)$, which is a product of single-site states of the form $\prod_j |\psi_j\rangle$, where $|\psi_j\rangle$ is defined by the equation

$$H_{ss}(j)\,|\psi_j\rangle = -(\sigma_z(j) + J\sigma_x(j))\,|\psi_j\rangle = -\sqrt{1+J^2}\,|\psi_j\rangle\,.$$

In this approximation it is possible to rewrite $Z(\delta)$ as

$$Z(\delta) = \left(e^{\delta\sqrt{1+J^2}}\cosh(\delta\lambda)\right)^V \left\langle \prod_j (1 + \tanh(\delta\lambda)\sigma_x(j)\,\sigma_x(j+1)) \right\rangle \tag{4.30}$$

To now this calculation parallels earlier ones. A new feature arises because $\langle\sigma_x(j)\rangle$ no longer vanishes. This means that it isn't possible to replace the expectation value in Eq. (4.30) by unity since in the current trial state

$$\langle\sigma_x(j)\rangle = f(J) = -J/\sqrt{1+J^2}.$$

To come as close to the original argument as possible one defines

$$\sigma'_x(j) = \sigma_x(j) - f(J)$$

and rewrites

$$Z(\delta) = \left(e^{\delta\sqrt{1+J^2}}\cosh(\delta\lambda)\right)^V \left\langle \prod_j (1 + \tanh(\delta\lambda)\,(\sigma'_x(j)\,\sigma'_x(j+1) + f(J)\sigma'_x(j) + f(J)\sigma'_x(j+1) + f(j)^2) \right\rangle \tag{4.31}$$

Factoring out an overall constant and rewriting Eq. (4.31) one obtains

$$Z(\delta) = \left(e^{\delta\sqrt{1+J^2}}\cosh(\delta\lambda)\,(1 + \tanh(\delta\lambda)\,f(J)^2)\right)^V \left\langle \prod_j (1 + \frac{\tanh(\delta\lambda)}{1 + \tanh(\delta\lambda)\,f(J)^2}(\sigma'_x(j)\,\sigma'_x(j+1) + f(J)\sigma'_x(j) + f(J)\sigma'_x(j+1)) \right\rangle \tag{4.32}$$

Introduction of $\sigma'_x(j)$ simplifies the evaluation of the expectation value since $\langle\sigma'_x(j)\rangle = 0$ and no term in the expansion of the product of operators containing $\sigma'_x(j)$ to the

first power can contribute. The first term which can appear is of the form

$$\left[\frac{\tanh(\delta\lambda)}{1+\tanh(\delta\lambda)\,f(J)^2}\right]^3 \left\langle\, [f(J)\sigma_x'(j)]\,[\sigma_x'(j)\,\sigma_x'(j+1)]\,[f(J)\sigma_x'(j+1)]\,\right\rangle \quad (4.33)$$

and comes from terms associated with the sites $j-1$, j and $j+1$. Since $\langle\sigma_x'(j)^2\rangle = 1-f(J)^2$ the lowest non-vanishing contribution to the expectation value, aside from unity, is

$$\left[\frac{\tanh(\delta\lambda)}{1+\tanh(\delta\lambda)\,f(J)^2}\right]^3 f(J)^2\,(1-f(J)^2)^2 \quad (4.34)$$

which vanishes when $f(J)$ is zero or unity. Since the factor $f(J)^2\,(1-f(J)^2)$ has a maximum value of $4/27$, this shows that the contribution of the lowest order symmetric approximation can be written as a product of non-trivial functions of δ times an expansion in a small parameter. Furthermore, since $f(J) = 0$ below the phase transition and is nearly unity a above the transition, it follows that the terms of this form can only be significant in the vicinity of the phase transition. One should also note that higher order terms in the expansion are of the form

$$\left[\frac{\tanh(\delta\lambda)}{1+\tanh(\delta\lambda)\,f(J)^2}\right]^{2+r} f(J)^2\,(1-f(J)^2)^{r+1} \quad (4.35)$$

and are smaller than the leading order term.

To simplify the discussion which follows set the expectation value in Eq. (4.32) to unity. A better calculation can be done to include the corrections. Doing this and taking the logarithmic derivative of $Z(\delta)$ yields

$$\mathcal{E}(J) = -\sqrt{1+J^2} - \lambda\tanh(\delta\lambda) - \frac{f(J)^2\lambda\,(1-\tanh^2(\delta\lambda))}{1+f(J)^2\tanh(\delta\lambda)} \quad (4.36)$$

To convert Eq. (4.36) to an estimate of the ground-state energy density for the Ising Hamiltonian note that if $|\psi(J)\rangle$ to denotes the exact ground-state of $H(J)$, then

$$\mathcal{E}(J) = \langle\psi(J)|\,H_{\rm Ising}\,|\psi(J)\rangle + J\sum_j \langle\psi(J)|\,\sigma_x(j)\,|\psi(J)\rangle \quad (4.37)$$

from which it follows that

$$\langle\psi(J)|\,H_{\rm Ising}\,|\psi(J)\rangle = \mathcal{E}(J) - J\sum_j \langle\psi(J)|\,\sigma_x(j)\,|\psi(J)\rangle \quad (4.38)$$

Since $|\psi(J)\rangle$ is not an exact eigenstate of $H_{\rm Ising}$ Eq. (4.38) provides and upper bound on the ground-state energy density of the Ising Hamiltonian, at least if

$\mathcal{E}(J)$ is a good estimate of the ground-state energy of $H(J)$. From this one sees that minimizing this expression with respect to the parameter J will produce a best bound on the ground-state energy density.

Henceforth I will refer to Eq. (4.38) as the "effective potential", $\Gamma(J)$, and use Eq. (4.36) to rewrite it as

$$\Gamma(J) = -\sqrt{1+J^2} - \lambda \tanh(\delta\lambda) - \frac{\lambda f(J)^2 (1 - \tanh^2(\delta\lambda))}{1 + f(J)^2 \tanh(\delta\lambda)} - J f(J) \tag{4.39}$$

Since, for the trial-state in question $f(J) = -J/\sqrt{1+J^2}$

$$\Gamma(J) = -\frac{1}{\sqrt{1+J^2}} - \lambda \tanh(\delta\lambda) - \lambda \left(\frac{J}{\sqrt{1+J^2}}\right)^2 \left(\frac{1 - \tanh^2(\delta\lambda)}{1 + J^2 \tanh(\delta\lambda)/(1+J^2)}\right) \tag{4.40}$$

Actually carrying out the minimization procedure for Eq. (4.40) will produce very strange results for large λ. As in the previous section, the solution to this problem is to rescale H_{Ising} so that only one term survives as $\lambda \to \infty$. In this case, however, the way to do this is to redefine

$$\begin{aligned} H(J) =& \frac{1}{\sqrt{1+J^2+\lambda^2}} \left[H_{\text{Ising}} + J \sum_j \sigma_x(j) \right] \\ & - \frac{1}{\sqrt{1+J^2+\lambda^2}} \sum_j \left[\sigma_z(j) + J\,\sigma_x(j) + \lambda\,\sigma_x(j)\,\sigma_x(j+1) \right] \end{aligned} \tag{4.41}$$

and multiply the expression for $\mathcal{E}(J)$ by $\sqrt{1+J^2+\lambda^2}$. With this modification the effective potential becomes

$$\Gamma(J) = -\frac{1}{\sqrt{1+J^2}} - \lambda \tanh(\delta'\lambda) - \lambda \left(\frac{J}{\sqrt{1+J^2}}\right)^2 \left(\frac{1 - \tanh^2(\delta'\lambda)}{1 + \frac{J^2}{1+J^2} \tanh(\delta'\lambda)}\right) \tag{4.42}$$

where $\delta' = \delta/\sqrt{1+J^2+\lambda^2}$.

In the limit $\delta = 0$,

$$\Gamma(J) = -\frac{1}{\sqrt{1+J^2}} - \lambda \left(\frac{J}{\sqrt{1+J^2}}\right)^2 \tag{4.43}$$

which is just the expectation value of H_{Ising} in a simple product state. In this limit $\Gamma(J)$ is a true bound on the ground-state energy density for H_{Ising} for all J.

Minimizing this bound with respect to J yields the usual mean-field prediction of a second-order phase transition at $\lambda = 1/2$. To simplify the derivation of this result it is customary to define

$$\begin{aligned} \sin(\alpha) &= \frac{J}{\sqrt{1+J^2}} \\ \cos(\alpha) &= \frac{1}{\sqrt{1+J^2}} \end{aligned} \tag{4.44}$$

and rewrite $\Gamma(J)$ as

$$\Gamma(\alpha) = -\cos(\alpha) - \lambda \tanh(\delta\lambda) - \lambda \sin^2(\alpha) \left(\frac{1 - \tanh^2(\delta\lambda)}{1 + \sin^2(\alpha) \tanh(\delta\lambda)} \right)$$

As promised, minimizing with respect to α yields

$$\sin(\alpha)(1 - 2\lambda \cos(\alpha)) = 0$$

which has a solution for non-vanishing α and therefore non-vanishing $\langle \sigma_x(j) \rangle$ if and only if $\lambda > 1/2$.

The same calculation for $\delta \neq 0$ is somewhat messier due to the more complicated dependence of Eq.(4.42) on J. Nevertheless, it is not difficult to determine the value of λ at which the phase transition occurs, since this point is the solution of the equation

$$1 - 2\lambda x = 0 \tag{4.45}$$

where

$$x = 1 - \tanh^2 \left(\frac{\delta\lambda}{\sqrt{1+\lambda^2}} \right) \tag{4.46}$$

Obviously, since $x \leq 1$ it follows that the location of the λ_c is greater than $1/2$. In fact, for $1 < \delta < 1.25$ we have $.67 \leq \lambda_c \leq 1.009$.

4.3.1 Comparison to Other Calculations

I already noted the simplest mean-field approximation to the Ising model predicts a second-order phase transition at $\lambda = 1/2$, which is quite far from the correct value of unity. Other attempts to improve upon this result fall into two classes: mean-field calculations based upon treating larger blocks exactly (i.e. block-mean-field calculations); attempts to combine the old t-expansion with the simple single-site mean-field calculations.

The calculation of a better effective potential using the old t-expansion does succeed in moving the value of λ_c closer to unity; however it requires working to high order in t and the use of Padé approximants introduces poles in J which make the extraction of final results problematic. While correct results can be extracted from these calculations there is the question of how obvious things would be if the exact answer was not known in advance.

Block-mean-field calculations [4] predict $\lambda_c > 1/2$, but $\lambda_c > .85$ is obtained only for blocks with more than eight sites. This sort of calculation involves considerably more work than the simple calculation just described. While taking $\delta \approx 1.2$ is suspect for a lowest-order symmetric approximation it is not out of the question for a calculation based upon two or three-site blocks, because for larger blocks more of the t-dependence is treated exactly. While carrying out a mean-field calculation for multi-site blocks is certainly more difficult than the one just described it is simpler than carrying out a naive t-expansion calculation or a block mean-field calculation for blocks of ten or more sites.

4.4 Adding The Hamiltonian Renormalization Group

The final topic I wish to touch upon is the combination of the symmetric expansion with Hamiltonian renormalization-group ideas. As with the discussion of the mean-field formalism I limit myself to a simple calculation which begins with the decomposition of H_{Ising} given in Eq. (4.21). I will limit myself to introducing the basic concepts and setting up the computational framework, I will not attempt to do an accurate treatment of the model.

4.4.1 Review of Hamiltonian Renormalization Group

The Hamiltonian real-space renormalizaton group procedure is a Rayleigh-Ritz calculation in which the trial-state is iteratively constructed. This section reviews the general method for the simple case of the Ising model to provide a framework for the discussion to follow. A more extensive discussion of these ideas can be found in Ref. 3.

The essential idea behind the Hamiltonian renormalization group procedure is to select from the set of all Hilbert-space states a smaller subset of states to be used to construct a "best" trial-state. Actually, instead of deciding which states to keep from the outset, the idea is to successively discard states in a multi-step procedure. Once one which states to discard it is necessary to recompute the matrix elements of the Hamiltonian in the remaining states. This produces a new *effective* Hamiltonian which has the same form as the original Hamiltonian but has

different values for the coupling constants. Thus, there are two steps in a procedure of this kind: the first, to decide, on some physical basis, which states to discard; the second, to compute the new effective or truncated Hamiltonian.

To see how this procedure works in detail consider the decomposition of the the Ising Hamiltonian specified in Eq. (4.21). Assume for the moment that the lattice has V sites. Since there are two states per site there are 2^V linearly independent states in the Hilbert space. The criteria use to select of a set of states to discard is based upon the intuitive notion that the lowest $2^{V/2}$ eigenstates of the sub-Hamiltonian

$$A = \sum_p H(p)$$

should have the biggest coefficients in the expansion of the ground-state of the full Ising Hamiltonian. These states are the ones spanned by taking tensor products of the lowest two-eigenstates of the two-site Hamiltonians $H(p)$. The eigenstates and eigenvalues of these Hamiltonians are shown in Table 2.

Having decided which states to keep imagine creating a general trial-state by adding up these states with arbitrary coefficients. Obviously computing the expectation value of the original Hamiltonian in such a variational state only requires knowledge of the matrix elements of H between any two states in this sub-space. It is simple to show that diagonalizing the *truncation* of the Ising Hamiltonian to this sub-space is equivalent to solving this general variational problem.

The computation of the truncated Hamiltonian is done in two steps. First compute the truncation of the operator A. As this operator is the sum of the $H(p)$ it suffices to compute the truncation of any one of the $H(p)$'s because they all have the same structure. The generic state we are keeping has the form

$$|\phi\rangle = \prod_p |\psi_p\rangle \tag{4.47}$$

where each of the $|\psi_p\rangle$'s is an eigenstate of the corresponding $H(p)$ which means that $H(p)$ is diagonal in this basis. In effect this means that these $2^{V/2}$ states can be thought of as belonging to a *new* spin theory defined on a lattice with half the number of sites. Since the new theory has two states for any site p and since the most general diagonal 2×2 matrix is a linear combination of the unit matrix and σ_z it is convenient to rewrite the truncation of $H(p)$ as

$$\Big[H(p)\Big]^T = -\Big(c_0 + \epsilon_0 \sigma_z'(p)\Big) \tag{4.48}$$

where $\sigma_z'(p)$ stands for a σ-matrix acting on the states of the new effective theory

and c_0 and ϵ_0 are given in terms of the eigenvalues of the two-site problem as

$$c_0 = \frac{1}{2}\left[\sqrt{4+\lambda^2}+\lambda\right]$$
$$\epsilon_0 = \frac{1}{2}\left[\sqrt{4+\lambda^2}-\lambda\right]$$

Thus

$$\Big[A\Big]^T = Vc_0 + \sum_p \epsilon_0 \sigma_z'(p)$$

The truncation of the operator B proceeds in a similar manner. Begin by observing that B is a sum of terms and it is only necessary to compute the truncation of one of the terms in the sum, since they all have the same structure. It is necessary, at this point, to note that the truncation of a product of operators which act on different blocks is the same as the product of the separately truncated operators; i.e.

$$\Big[\sigma_x(2p+1)\,\sigma_x(2(p+1))\Big]^T = \Big[\sigma_x(2p+1)\Big]^T \Big[\sigma_x(2(p+1))\Big]^T$$

Inspection of the entries in Table 2 shows that

$$\Big[\sigma_x(2p)\Big]^T = \Big[\sigma_x(2p+1)\Big]^T = \frac{\cos(\theta)+\sin(\theta)}{\sqrt{2}}\,\sigma_x'(p)$$

and so

$$\Big[B\Big]^T = -\sum_p \lambda' \sigma_x'(p)\,\sigma_x'(p+1)$$

where

$$\lambda' = \left[\frac{\cos(\theta)+\sin(\theta)}{\sqrt{2}}\,\sigma_x'(p)\right]^2 \lambda$$

Taken together these results show that, up to an additive constant, the truncated Hamiltonian can be rewritten as a Hamiltonian of the same general form but defined on a lattice with half as many sites. Clearly, this same procedure can be repeated, with only minor modifications, ad infinitum. The result of carrying out such a calculation is that for λ larger than some critical value, λ_c, the Hamiltonian iterates to one in which the coefficient of the $\sigma_z(p)$'s vanishes, whereas for $\lambda < \lambda_c$ the coefficient of the operators $\sigma_x(p)\,\sigma_x(p+1)$ iterates to zero. Of course, when this happens the resulting Hamiltonian can be solved exactly.

I already noted that the lowest eigenstate of a truncated Hamiltonian provides a variational upper bound on the ground-state of the original theory. From this it follows that the lowest eigenstate of the limiting Hamiltonian defines a best trial-state within the context of this general approximation scheme. Since a Hamiltonian of the form $\sum \sigma_z(p)$ has a unique ground-state, whereas one of the form $\sum \sigma_x(p)\,\sigma_x(p+1)$ has two degenerate ground-states, this variational calculation predicts very different symmetry properties for the ground-state of the original theory depending upon whether $\lambda > \lambda_c$ or $\lambda < \lambda_c$. In other words the real-space renormalization group calculation provides another way of determining the location of the phase transition in the original 1+1-dimensional Ising model. It is a simple matter to carry out the naive calculation just described and if one does so one obtains a value for $\lambda_c \approx .73$. There is a long history of attempts to significantly improve upon this result by working with larger blocks or by keeping more states in the truncation procedure, however the process quickly becomes very difficult without a corresponding increase in accuracy. Attempts to combine this procedure with the ordinary t-expansion quickly run into difficulties with both the complexity of the calculations involved and in the use of Padé approximants. In the next section I will show how to implement this simplest renormalization-group procedure within the framework of the lowest-order symmetric expansion and discuss the way in which the location of the critical point changes with increasing δ.

4.4.2 Truncation of the Symmetric Approximation

The calculation presented in section ? involves two distinct steps: rewriting the operator $e^{-\delta H}$ as a product $e^{-\delta A/2}\,e^{-\delta B}\,e^{-\delta A/2}$; choosing a trial-state in which to compute the operator expectation value. It is the second step which must be modified in order to incorporate the real-space renormalization group concept into the symmetric approximation scheme. Once again, the basic idea is to iteratively construct a variational wave-function to maximize the expectation value of $e^{-\delta H}$ and therefore minimize the expectation value of H. As in the preceding discussion it is not necessary to commit to a specific wave-function in advance; one can instead successively prune away unwanted states and compute a series of truncations of $e^{-\delta H}$.

In what follows I limit myself to the lowest order symmetric approximation, although the method generalizes to higher-order approximation quite nicely. Since the operator A which appears in Eq. (4.21) is a sum of commuting operators it is

always possible to rewrite the two exponentials as

$$\begin{aligned} e^{-\delta A/2} &= \prod_p e^{\frac{1}{2}\delta'\left(\sigma_z(2p)+\sigma_z(2p+1)+\lambda\sigma_x(2p)\,\sigma_x(2p+1)\right)} \\ &= \prod_p e^{A_p} \\ e^{-\delta B} &= \prod_p \Big(\cosh(\delta'\lambda) + \sinh(\delta'\lambda)\,\sigma_x(2p+1)\,\sigma_x(2(p+1)) \Big) \end{aligned} \tag{4.49}$$

where δ' is defined to be $\delta' = \delta/\sqrt{1+\lambda^2}$ in order to include, as in earlier discussions, the rescaling of the Hamiltonian by an overall factor $\sqrt{1+\lambda^2}$. The truncation step introduced in the previous section is equivalent to restricting attention to the $2^{V/2}$-dimensional space of states generated by taking products over p of the two eigenvectors of e^{A_p} having the largest eigenvalues. Since the different factors e^{A_p} commute with one another and are diagonal in this space of states the truncation of the lowest symmetric approximation becomes

$$\prod_{p_1}\Big(\alpha+\beta\,\sigma_z'(p_1)\Big)\Big[\prod_{p_2}\Big(\cosh(\delta'\lambda)+\sinh(\delta'\lambda)\,\sigma_x(2p_2+1)\,\sigma_x(2(p_2+1))\Big)\Big]^T \prod_{p_3}\Big(\alpha+\beta\,\sigma_z'(p_3)\Big) \tag{4.50}$$

where there is still the problem of computing the truncation of the product over p_2. The simplest way to understand the truncation of this product is to rewrite it as the truncation of an exponential, compute the truncation of the Taylor series expansion of this operator and then take the logarithm of the resulting expression. More precisely, rewrite

$$\prod_p \Big(\cosh(\delta'\lambda) + \sinh(\delta'\lambda)\,\sigma_x(2p+1)\,\sigma_x(2(p+1)) \Big) = e^{\delta'\lambda\sum_p \sigma_x(2p+1)\,\sigma_x(2(p+1))} \tag{4.51}$$

and expand the exponential to obtain

$$\begin{aligned} \Big[e^{\delta'\lambda\sum_p \sigma_x(2p+1)\,\sigma_x(2(p+1))}\Big]^T &= 1+\delta'\lambda\sum_p\Big[\sigma_x(2p+1)\,\sigma_x(2(p+1))\Big]^T \\ &+\frac{(\delta'\lambda)^2}{2}\sum_{p_1,p_2}\Big[\sigma_x(2p_1+1)\,\sigma_x(2(p_1+1))\,\sigma_x(2p_2+1)\,\sigma_x(2(p_2+1))\Big]^T \\ &+\ldots \end{aligned} \tag{4.52}$$

Operators which do not lie in the same block can be truncated independently of

one another and so, if $p_1 \neq p_2$ or $p_1 \neq p_2 \pm 1$ then

$$\Big[\sigma_x(2p_1+1)\,\sigma_x(2(p_1+1))\,\sigma_x(2p_2+1)\,\sigma_x(2(p_2+1))\Big]^T = \Big[\sigma_x(2p_1+1)\,\sigma_x(2(p_1+1))\Big]^T\Big[\sigma_x(2p_2+1)\,\sigma_x(2(p_2+1))\Big]^T$$

If $p_1 = p_2$ then the product is the identity operator whose truncation is the identity operator; so this term contributes

$$\frac{1}{2}(\delta'\,\lambda)^2\sum_p \mathbf{1}_p$$

Finally, if $p_2 = p_1 + 1$ then

$$\Big[\sigma_x(2p_1+1)\,\sigma_x(2(p_1+1))\,\sigma_x(2(p_1+1)+1)\,\sigma_x(2(p_2+1))\Big]^T = \Big[\sigma_x(2p_1+1)\Big]^T\Big[\sigma_x(2(p_1+1))\sigma_x(2(p_1+1)+1)\Big]^T\Big[\sigma_x(2(p_1+2))\Big]^T$$

a similar expression holds for $p_2 = p_1 - 1$. Taking the logarithm of Eq.(4.52) we see that except for $p_1 = p_2$ and $p_1 = p_2 \pm 1$ all of the contributions cancel so that finally

$$\begin{aligned}\log\Big[e^{\delta'\lambda\sum_p \sigma_x(2p+1)\,\sigma_x(2(p+1))}\Big]^T &= \delta'\,\lambda\sum_p\Big[\sigma_x(2p+1)\Big]^T\Big[\sigma_x(2(p+1))\Big]^T \\ &+\frac{1}{2}(\delta'\,\lambda)^2\sum_p\left(\mathbf{1}_p-\left(\Big[\sigma_x(2p+1)\Big]^T\Big[\sigma_x(2(p+1))\Big]^T\right)^2\right) \\ &+(\delta'\,\lambda)^2\sum_p\Big[\sigma_x(2p+1)\Big]^T\Big(\Big[\sigma_x(2(p+1))\,\sigma_x(2(p+1)+1)\Big]^T \\ &-\Big[\sigma_x(2(p+1))\Big]^T\Big[\sigma_x(2(p+1)+1)\Big]^T\Big)\Big[\sigma_x(2(p+2))\Big]^T \\ &+\ldots\end{aligned} \tag{4.53}$$

It is important to note is that the second term of order $(\delta'\,\lambda)^2$ is part of a linked cluster expansion, all of whose terms have a similar structure. This term, which is

proportional to the difference between the truncation of

$$\left[\sigma_x(2(p+1))\,\sigma_x(2(p+1)+1)\right]^T$$

and

$$\left[\sigma_x(2(p+1))\right]^T\left[\sigma_x(2(p+1)+1)\right]^T$$

is a generalization of the terms which appeared in the discussion of the mean-field approximation. As in the case of the mean-field calculation it is small, except in the vicinity of the phase transition. Far below the transition $\delta \ll 1$, whereas well above the transition $\delta >> 1$ and the difference of truncations nearly vanishes. More precisely, since

$$\begin{aligned}
\left[\sigma_x(2p)\right]^T &= \frac{\cos(\theta)+\sin(\theta)}{\sqrt{2}}\,\sigma'_x(p) \\
\left[\sigma_x(2p+1)\right]^T &= \frac{\cos(\theta)+\sin(\theta)}{\sqrt{2}}\,\sigma'_x(p) \\
\left[\sigma_x(2p)\,\sigma_x(2p+1)\right]^T &= \frac{1+\sin(2\theta)}{2}+\frac{-1+\sin(2\theta)}{2}\,\sigma'_z(p)
\end{aligned} \tag{4.54}$$

this difference is equal to

$$\frac{\sin(2\theta)-1}{2}\,\sigma'_z(p)$$

where $\tan(\theta) = (\sqrt{4+\lambda^2}-2)/\lambda$. Thus, for $\lambda \ll 1$ the order $(\delta'\lambda)^2$ is of the form $-(\delta^2\lambda^2/8)\sigma'_x(p)\,\sigma'_z(p+1)\,\sigma'_x(p+1)$ whereas for $\lambda >> 1$ the operator is $-(1/2\lambda^2)\,\sigma'_x(p)\,\sigma'_z(p+1)\,\sigma'_x(p+1)$. In either case, as with the mean-field calculation, this term has a small coefficient and the higher-order terms are suppressed and can be ignored to zeroth approximation, as they can be included in a later calculation. Ignoring these terms and factoring out the term proportional to the unit operator, the first truncation of the lowest-order symmetric approximation becomes

$$\begin{aligned}
&e^{\frac{1}{2}(\delta'\lambda)^2\left(1-\frac{1}{4}(\cos(\theta)+\sin(\theta))^4\right)}\prod_{p_1}\Big(\alpha+\beta\,\sigma'_z(p_1)\Big) \\
&\qquad\prod_{p_2}\Big(\cosh(\tau)+\sinh(\tau)\,\sigma'_x(p_2)\,\sigma'_x(p_2+1)\Big)\prod_{p_3}\Big(\alpha+\beta\,\sigma'_z(p_3)\Big)
\end{aligned} \tag{4.55}$$

where $\tau = \delta\,\lambda\,(\sin(\theta)+\cos(\theta))/2\sqrt{1+\lambda^2}$

At this point the truncation of the symmetric expansion has the same general form as the original expression; i.e., this truncation step can be thought of as a renormalization-group transformation. Since the form of the product is the same as before one can iterate the procedure by defining

$$U_p = \left(\cosh(\tau/2) + \sinh(\tau/2)\, \sigma_x'(2p)\, \sigma_x'(2p+1) \right) \left(\alpha + \beta\, \sigma_z'(2p) \right) \left(\alpha + \beta\, \sigma_z'(2p+1) \right)$$

and rewriting Eq. (4.55) as

$$\prod_{p_1} U_{p_1}^{\dagger} \prod_{p_2} \left(\cosh(\tau) + \sinh(\tau)\, \sigma_x'(2p_2+1)\, \sigma_x'(2(p_2+1)) \right) \prod_{p_3} U_{p_3} \qquad (4.56)$$

The generic truncation step is to then to limit oneself to the subspace generated by products of the two highest of U_p. Once again the truncation of any U_p is of the form of a number times the unit matrix plus another number times $\sigma_z'(p)$ and the truncation of the block-block recoupling terms proceeds as before.

As in the naive Hamiltonian real-space renormalization group approach the idea is to study the flows of the matrices

$$U_p \text{and} \left(\cosh(\tau) + \sinh(\tau)\, \sigma_x'(2p)\, \sigma_x'(2p+1) \right)$$

and determine the location of the critical point. The ground-state energy is reconstructed from the constant factors which accumulate with each step of the renormalization-group procedure.

4.4.3 Comparison To Other Calculations

The results of this calculation are quite striking when compared to those obtained from the naive Hamiltonian renormalization group or the operator t-expansion5. As expected, in the limit $\delta = 0$, the analysis agrees with the results of the naive Hamiltonian renormalization-group calculation, $\lambda_c \approx .78$, but this value increases towards unity with increasing δ. For values of $\delta > .7$ the location of the phase transition is greater than .93, which is better than the results obtained for the mean-field calculation which required working to order t^7 and larger values of δ. This is not really surprising since the renormalization-group procedure is capable of producing a much better starting wave-function. To achieve this kind accuracy using the much more complicated t-expansion approach to the renormalization-group required working to at least t^5 and tuning a free parameter in the reconstruction procedure.

5. Conclusions

I have only scratched the surface of what can be done using the higher-order symmetric approximation scheme to organize lattice spin-system and field-theory computations. While I touched upon the way in which one can extract the properties of the 1+1-dimensional Ising model, I did not discuss the pedagogically interesting question of how to derive, for $\lambda > 1$, closed expressions for the mixing of the two would-be vacuum states when working in finite volume; nor did I talk about the simple picture which emerges of the important role played by solitons in this tunneling process. Furthermore, while I discussed the mechanics of the Hamiltonian renormalization group process and the way in which one can improve these calculations, I did not present a detailed discussion of why this formalism does so much better for a given amount of work. Given the length of this document I decided that these largely pedagogical points were better put off to another paper.

While I believe that this paper shows that the symmetric approximation scheme suggests many possible ways of attacking non-perturbative problems, much work remains to be done to see just how far one can get with more interesting examples both in one, two and three space dimensions. The application of these ideas to anti-ferromagnets and Hubbard models are of particular interest. While the addition of fermions to the scheme poses no particular problems, it remains to be seen if the subtleties of such models can be easily extracted using the tools presented. Furthermore, although interesting possibilities for carrying out calculations in lattice-gauge systems suggest themselves, detailed calculations have yet to be carried out and it remains to be seen how they will compare to results obtained from strong-coupling expansions, high order t-expansions and Monte-Carlo calculations. Preliminary study of these questions show that, as for the cases studied in this paper, heretofore puzzling aspects of t-expansion, Padé approximants and Hamiltonian renormalization group calculations become easier to understand. Also, the same analysis shows there are many fewer terms at each order than for the corresponding t-expansion. This suggests that MapleV, the computer algebra program used for these calculations, will be able to handle computations in the more interesting cases as well.

APPENDIX A

Since the general derivation of the higher-order symmetric expansions leads to formulae which cannot be easily evaluated beyond terms of order δ^3 I begin by giving explicit forms for the expansions used in the body of the paper. The formula for the simplest symmetric expansion of a sum of two operators is given by

$$e^{-\delta(A+B)} = e^{-\delta A/2}\, e^{-\delta B/2}\, e^{C_3(\delta)}\, e^{-\delta B/2}\, e^{-\delta A/2} \tag{A.1}$$

where the operator $C_3(\delta)$ can be written as

$$C_3(\delta) = \sum_{n=1}^{\infty} \delta^{2n+1} O_{2n+1} \tag{A.2}$$

Up to and including terms of order δ^7 we have

$$\begin{aligned}
C_3(\delta) = &-\delta^3 \left(\frac{1}{12}[B,[A,B]] + \frac{1}{24}[A,[A,B]] \right) \\
&-\delta^5 \left(\frac{1}{480}[B,[A,[A,[A,B]]]] - \frac{1}{480}[[A,B],[A,[A,B]]] \right. \\
&\quad + \frac{1}{320}[B,[B,[A,[A,B]]]] - \frac{1}{240}[[A,B],[B,[A,B]]] \\
&\quad \left. + \frac{1}{1920}[A,[A,[A,[A,B]]]] + \frac{1}{480}[B,[B,[B,[A,B]]]] \right) \\
&-\delta^7 \left(\frac{1}{21504}[B,[B,[B,[B,[A,[A,B]]]]]] - \frac{1}{13440}[[A,B],[B,[B,[B,[A,B]]]]] \right. \\
&\quad + \frac{1}{2688}[[B,[A,B]],[B,[B,[A,B]]]] + \frac{1}{16128}[B,[B,[B,[A,[A,[A,B]]]]]] \\
&\quad - \frac{1}{8960}[[A,B],[B,[B,[A,[A,B]]]]] + \frac{1}{2688}[[B,[A,B]],[B,[A,[A,B]]]] \\
&\quad + \frac{1}{5376}[[A,[A,B]],[B,[B,[A,B]]]] + \frac{1}{21504}[B,[B,[A,[A,[A,[A,B]]]]]] \\
&\quad \left. + \frac{1}{53760}[B,[B,[B,[B,[B,[A,B]]]]]] - \frac{1}{13440}[[A,B],[B,[A,[A,[A,B]]]]] \right)
\end{aligned}$$

$$+\frac{1}{8064}[[B,[A,B]],[A,[A,[A,B]]]]+\frac{1}{13440}[[A,B],[[A,B],[A,[A,B]]]]$$
$$+\frac{1}{53760}[B,[A,[A,[A,[A,[A,B]]]]]]-\frac{1}{53760}[[A,B],[A,[A,[A,[A,B]]]]]$$
$$+\frac{1}{16128}[[A,[A,B]],[A,[A,[A,B]]]]+\frac{1}{5376}[[A,[A,B]],[B,[A,[A,B]]]]$$
$$+\frac{1}{322560}[A,[A,[A,[A,[A,[A,B]]]]]]+\frac{1}{6720}[[A,B],[[A,B],[B,[A,B]]]]\Big) \tag{A.3}$$

The formula for a sum of three operators is

$$e^{-\delta(A+B+C)}=e^{-\delta A/2}\,e^{-\delta B/2}\,e^{-\delta C/2}\,e^{C_3'(\delta)}\,e^{-\delta C/2}\,e^{-\delta B/2}\,e^{-\delta A/2} \tag{A.4}$$

where, up to and including terms of order δ^5 we have

$$C_3'(\delta)=-\delta^3\Big(\frac{1}{24}[A,[A,B]]+\frac{1}{24}[A,[A,C]]+\frac{1}{12}[B,[A,B]]$$
$$+\frac{1}{12}[B,[A,C]]+\frac{1}{24}[B,[B,C]]+\frac{1}{12}[C,[A,B]]$$
$$+\frac{1}{12}[C,[A,C]]+\frac{1}{12}[C,[B,C]]\Big)$$
$$-\delta^5\Big(\frac{1}{320}[C,[C,[A,[A,B]]]]-\frac{1}{240}[[A,C],[B,[A,C]]]-\frac{1}{480}[[B,C],[B,[B,C]]]$$
$$-\frac{1}{240}[[A,C],[C,[A,B]]]+\frac{1}{480}[C,[B,[B,[B,C]]]]+\frac{1}{160}[C,[B,[A,[A,C]]]]$$
$$-\frac{1}{240}[[B,C],[B,[A,C]]]+\frac{1}{480}[C,[C,[C,[A,B]]]]+\frac{1}{480}[C,[C,[C,[B,C]]]]$$
$$+\frac{1}{480}[C,[C,[C,[A,C]]]]-\frac{1}{240}[[A,B],[C,[A,C]]]-\frac{1}{480}[[A,B],[B,[B,C]]]$$
$$+\frac{1}{1920}[B,[B,[B,[B,C]]]]+\frac{1}{480}[B,[B,[B,[A,C]]]]+\frac{1}{160}[C,[B,[B,[A,B]]]]$$
$$+\frac{1}{240}[[B,[A,B]],[B,C]]+\frac{1}{480}[B,[B,[B,[A,B]]]]+\frac{1}{480}[B,[A,[A,[A,C]]]]$$
$$-\frac{1}{240}[[A,B],[B,[A,B]]]+\frac{1}{320}[B,[B,[A,[A,B]]]]-\frac{1}{480}[[B,C],[A,[A,C]]]$$
$$-\frac{1}{480}[[A,C],[A,C[A,C]]]+\frac{1}{480}[C,[A,[A,[A,C]]]]-\frac{1}{240}[[A,B],C[C,[A,B]]]$$

$$
\begin{aligned}
&-\frac{1}{480}[[B,C],[A,[A,B]]]+\frac{1}{160}[C,[B,[A,[A,B]]]]+\frac{1}{240}[[B,[A,B]],[A,C]]\\
&-\frac{1}{240}[[B,C],[C,[B,C]]]+\frac{1}{320}[B,[B,[A,[A,C]]]]-\frac{1}{240}[[A,B],[B,[A,C]]]\\
&+\frac{1}{320}[C,[C,[B,[B,C]]]]+\frac{1}{480}[B,[A,[A,[A,B]]]]-\frac{1}{480}[[A,B],[A,[A,B]]]\\
&+\frac{1}{480}[C,[A,[A,[A,B]]]]-\frac{1}{480}[[A,B],[A,[A,C]]]-\frac{1}{480}[[A,C],[A,[A,B]]]\\
&+\frac{1}{1920}[A,[A,[A,[A,B]]]]+\frac{1}{1920}[A,[A,[A,[A,C]]]]+\frac{1}{160}[C,[B,[B,[A,C]]]]\\
&-\frac{1}{240}[[A,B],[C,[B,C]]]-\frac{1}{240}[[B,C],[C,[A,B]]]-\frac{1}{480}[[A,C],[B,[B,C]]]\\
&+\frac{1}{320}[C,[C,[A,[A,C]]]]-\frac{1}{240}[[A,C],[C,[A,C]]]-\frac{1}{240}[[B,C],[C,[A,C]]]\\
&-\frac{1}{240}[[A,C],[C,[B,C]]]+\frac{1}{160}[C,[C,[B,[A,B]]]]+\frac{1}{160}[C,[C,[B,[A,C]]]]\Big)
\end{aligned}
$$

The derivations of formulae of this type all follow the same general pattern. While, as I have already noted, the formulae one derives in this way can be difficult to use, it is useful to understand the ideas behind the derivation to appreciate why the statements made in the body of this paper are valid. I will now sketch the derivation for the simplest case of the sum of two operators.

The symmetric expansion for a sum of two non-commuting operators requires that we find an operator $C_3(\delta)$ such that

$$
e^{\delta(A+B)} = e^{\frac{\delta}{2}A}\, e^{\frac{\delta}{2}B}\, e^{C_3(\delta)}\, e^{\frac{\delta}{2}B}\, e^{\frac{\delta}{2}A}
$$

Equivalently, by multiplying both sides of this equality by by $e^{-\frac{\delta}{2}B}\, e^{-\frac{\delta}{2}A}$ on the left and $e^{-\frac{\delta}{2}A}\, e^{-\frac{\delta}{2}B}$ we can convert it to

$$
e^{C_3(\delta)} = e^{-\frac{\delta}{2}B}\, e^{-\frac{\delta}{2}A}\, e^{\delta(A+B)}\, e^{\frac{-\delta}{2}A}\, e^{-\frac{\delta}{2}B}
$$

Expanding the exponentials on the right-hand side of the equation yields

$$
e^{C_3(\delta)} = \sum_{j,k,l,m,n=0}^{\infty} (-1)^{j+k+m+n}\, \delta^{j+k+l+m+n}\, \frac{B^j\, A^k\, (A+B)^l\, A^m\, B^n}{j!\, k!\, l!\, m!\, n!}
$$

and taking the logarithm of both sides we arrive at

$$
\begin{aligned}
C_3(\delta) = \sum_{\substack{r,j_1,k_1,l_1,m_1,n_1\ldots\\ j_r,k_r,l_r,m_r,n_r}} & (-1)^{p_r}\, \delta^{q_r}\\
& \frac{B^{j_1}\, A^{k_1}\, (A+B)^{l_1}\, A^{m_1}\, B^{n_1} \ldots B^{j_r}\, A^{k_r}\, (A+B)^{l_r}\, A^{m_r}\, B^{n_r}}{r j_1!\, k_1!\, l_1!\, m_1!\, n_1! \ldots j_r!\, k_r!\, l_r!\, m_r!\, n_r!}
\end{aligned}
\tag{A.5}
$$

where

$$p_r = r + j_1 + k_1 + m_1 + n_1 + \ldots + j_r + k_r + m_r + n_r$$
$$q_r = j_1 + k_1 + l_1 + m_1 + n_1 + \ldots + j_r + k_r + l_r + m_r + n_r$$

While, with great effort, one could manipulate this expression into a sum of multiple commutators, there is a trick which simplifies this task. This trick is based upon the observation that the mapping

$$O_1 O_2 \ldots O_n \rightarrow \frac{1}{n}[O_1, [O_2, [O_3 \ldots [O_{n-1}, O_n]] \ldots]$$

which takes a formal product of n operators into a multiple commutator, in other words a member of the lie algebra, is the identity mapping when applied to something which is already in the Lie algebra. This statement assumes, of course, that the basic mapping is extended to a sum of products by linearity. Thus, for example,

$$O_1 O_2 - O_2 O_1 \rightarrow \frac{1}{2}[O_1, O_2] - \frac{1}{2}[O_2, O_1] = [O_1, O_2]$$

Since one knows that Eq. (A.5) can be be expressed as a sum of commutators, it follows that every term in the sum appearing on the right hand side of the expression can be independently mapped into a sum of commutators. Of course this means that terms which have more than one power of A or B as the right-most factor in a summand vanish identically.

As I already noted, the formula which one obtains in this way is difficult to work with. In practice I have found that the simplest way to generate higher-order terms is to teach an symbolic math program, in my case MapleV, to do the explicit multiplication of finite power-series and then simplify the result by applying the mapping defined above to the result.

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[5] The notion of combining the t-expansion with the Hamiltonian real-space renormalization group method was introduced in David Horn, W.G.J. Langeveld, Helen R. Quinn, Marvin Weinstein,, *Phys.Rev.* **D38**, 3238 (1988), and was applied to spin systems in C. Stubbins,, *Phys.Rev.* **D44**, 488 (1991),

[6] After completing this paper I became aware of the paper by Masuo Suzuki,, *Physics Letter* **A 165**, 387 (1992), which gives an extensive treatment of the derivation of formulae such as the higher-order symmetric expansions. The results of this paper are quite general and the derivation follows the general form given in the appendix.

TABLE CAPTIONS

1: Computation of Feynman and symmetric approximation

2: Table of eigenvectors and eigenvalues for H_p

FIGURE CAPTIONS

1) A plot of $\mathcal{E}(\delta)$ computed for $\gamma = 1$, for each of the approximations compared to the exact answer of $1/2$.

2) A plot of $\mathcal{E}(\delta)$ computed for $\gamma = 2$, for each of the approximations.

3) A plot of the exact ground-state energy and the simplest approximation based on the lowest order symmetric approximation for $\delta = .5, 1, 5$.

4) A plot of the exact ground-state energy and the simplest approximation based on the lowest order symmetric approximation for $\delta = .5, 1, 5.$ for the rescaled Hamiltonian

5) A plot of the exact ground-state energy versus the 2-site lowest order approximation for various values of δ

δ	Feynman Approx	% Error	First Symmetric	% Error	High Order Symmetric	% Error
0.00	.50000000	0	.50000000	0	.50000000	.000000000
0.01	.49997525	.00004950	.49999375	.00001250	.50000000	.000000000
0.02	.49990198	.00019604	.49997500	.00004998	.50000000	.000000000
0.03	.49978165	.00043670	.49994377	.00011245	.50000000	.000000000
0.04	.49961568	.00076863	.49990007	.00019984	.50000000	.000000000
0.80	.42452830	.15094339	.46703296	.06593406	.50002433	.000048671
0.90	.41214751	.17570498	.45985706	.08028587	.50009010	.000180207
1.00	.40000000	.20000000	.45238095	.09523809	.50028167	.000563348
1.10	.38817006	.22365988	.44469113	.11061773	.50077556	.001551121
1.40	.35502959	.28994082	.42103142	.15793714	.50946778	.018935569
1.50	.34482759	.31034482	.41312741	.17374517	.51906299	.038125996

Table I

Eigenvector	Eigenvalue
$\|\uparrow'\rangle = \cos(\theta)\ \|\uparrow\uparrow\rangle + \sin(\theta)\ \|\downarrow\downarrow\rangle$	$-\sqrt{4+\lambda^2}$
$\|\downarrow'\rangle = \frac{1}{\sqrt{2}}\left(\|\uparrow\downarrow\rangle + \|\downarrow\uparrow\rangle\right)$	$-\lambda$
$\frac{1}{\sqrt{2}}\left(\|\uparrow\downarrow\rangle - \|\downarrow\uparrow\rangle\right)$	λ
$-\sin(\theta)\ \|\uparrow\uparrow\rangle + \cos(\theta)\ \|\downarrow\downarrow\rangle$	$\sqrt{4+\lambda^2}$
where $\tan(\theta) = \left(\sqrt{4+\lambda^2} - 2\right)/\lambda$	

Table II

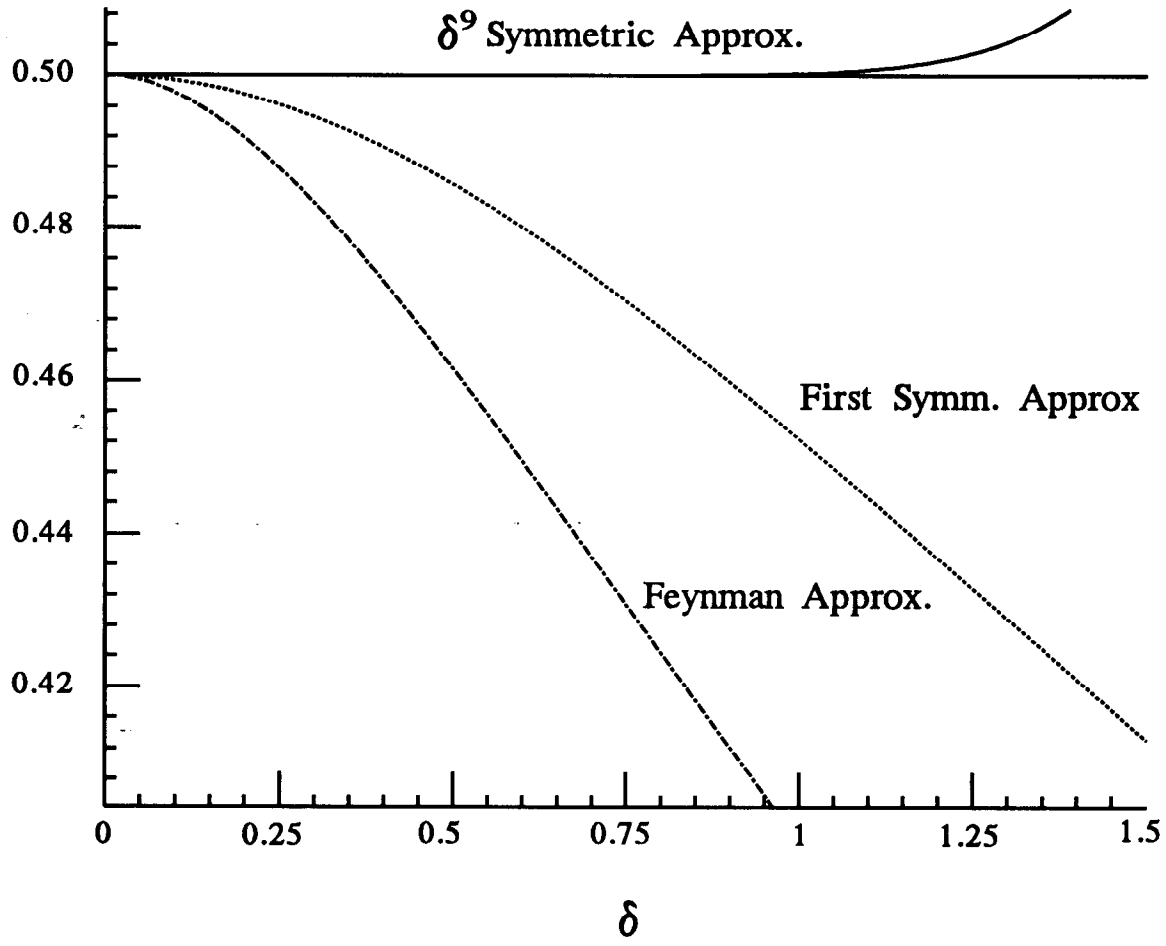
δ^9 Symmetric Approx.
0.50
0.48
0.46
0.44
0.42
First Symm. Approx
Feynman Approx.
0
0.25
0.5
0.75
1
1.25
1.5
δ

Fig 1

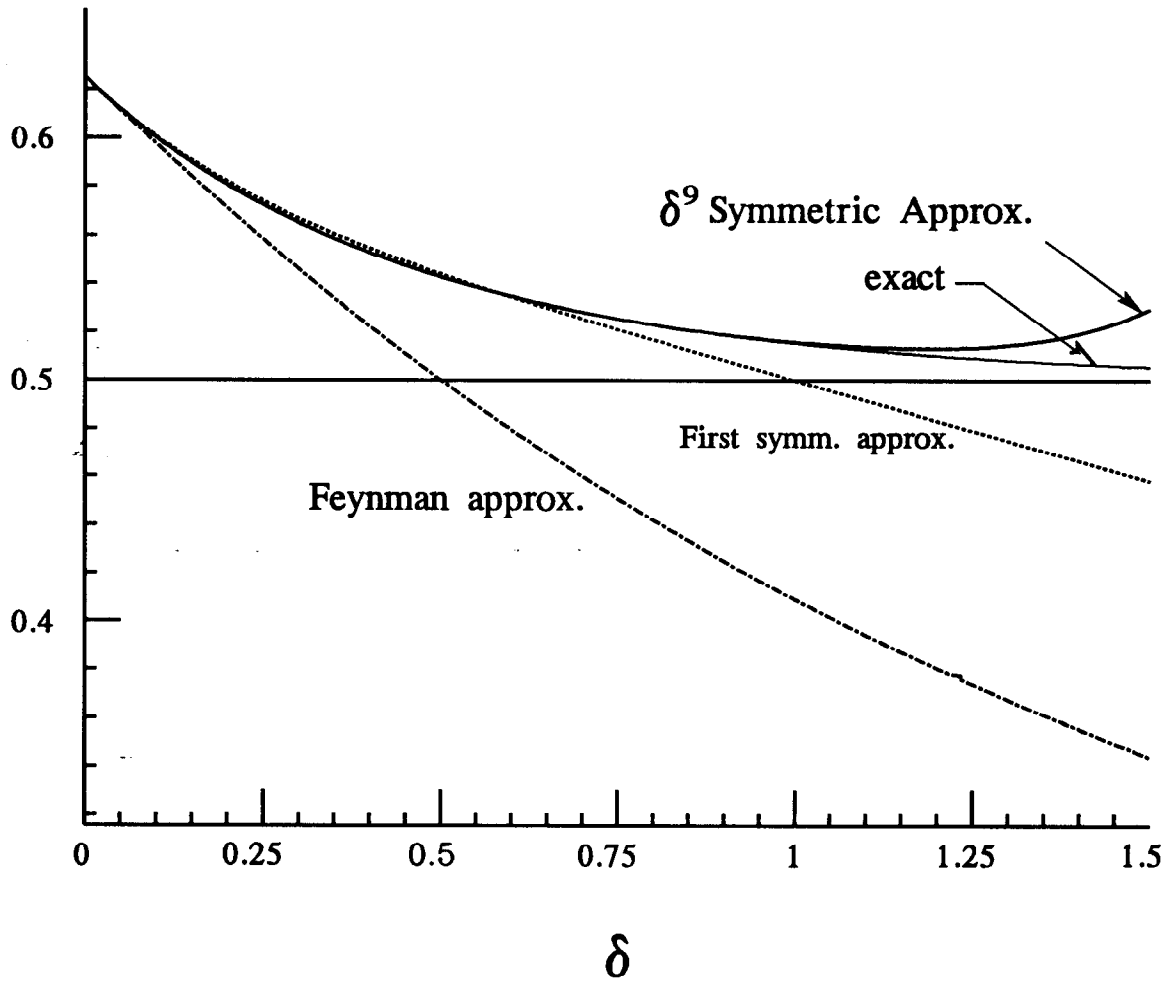
0.6
0.5
0.4
δ^9 Symmetric Approx.
exact
First symm. approx.
Feynman approx.
0
0.25
0.5
0.75
1
1.25
1.5
δ

Fig. 2

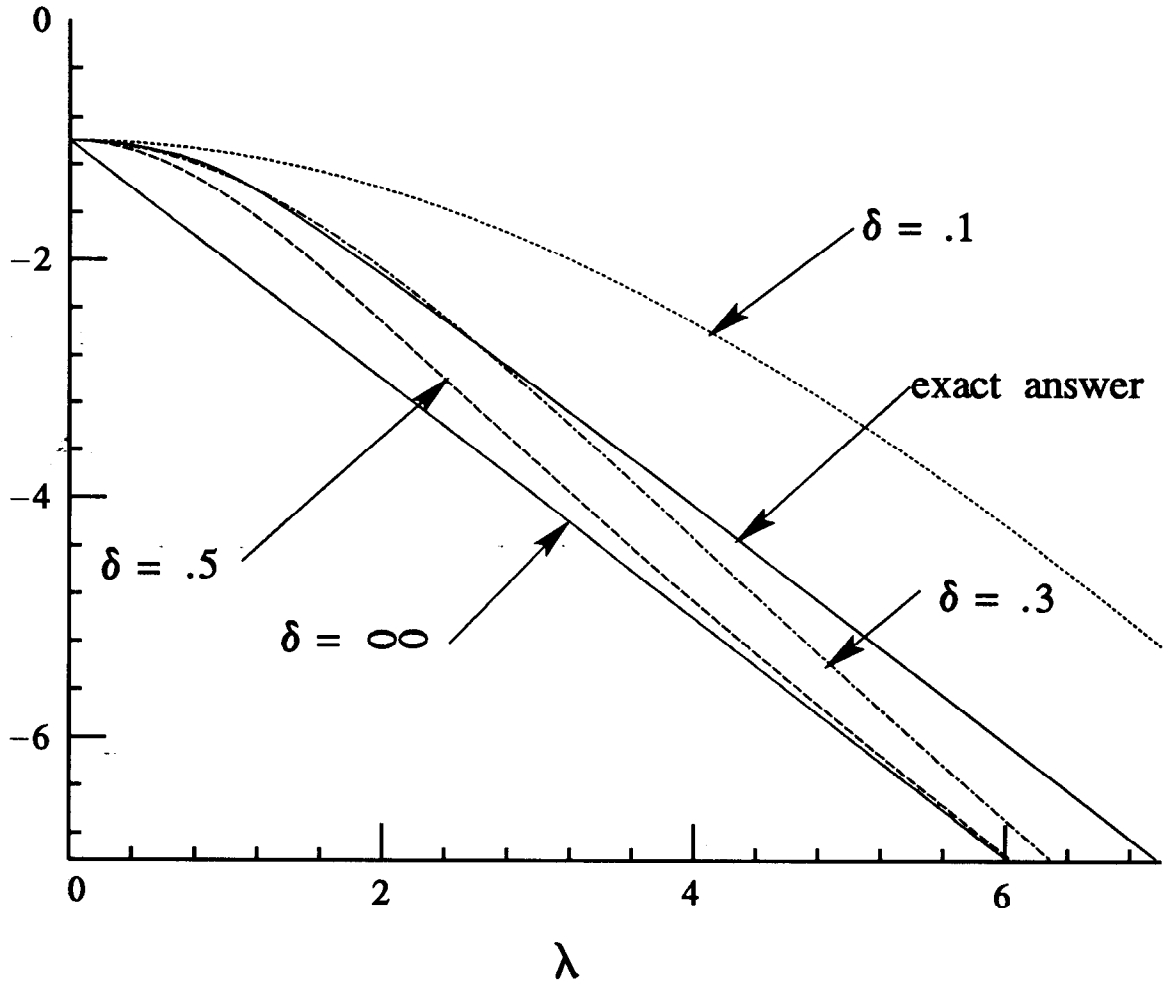

Fig. 3

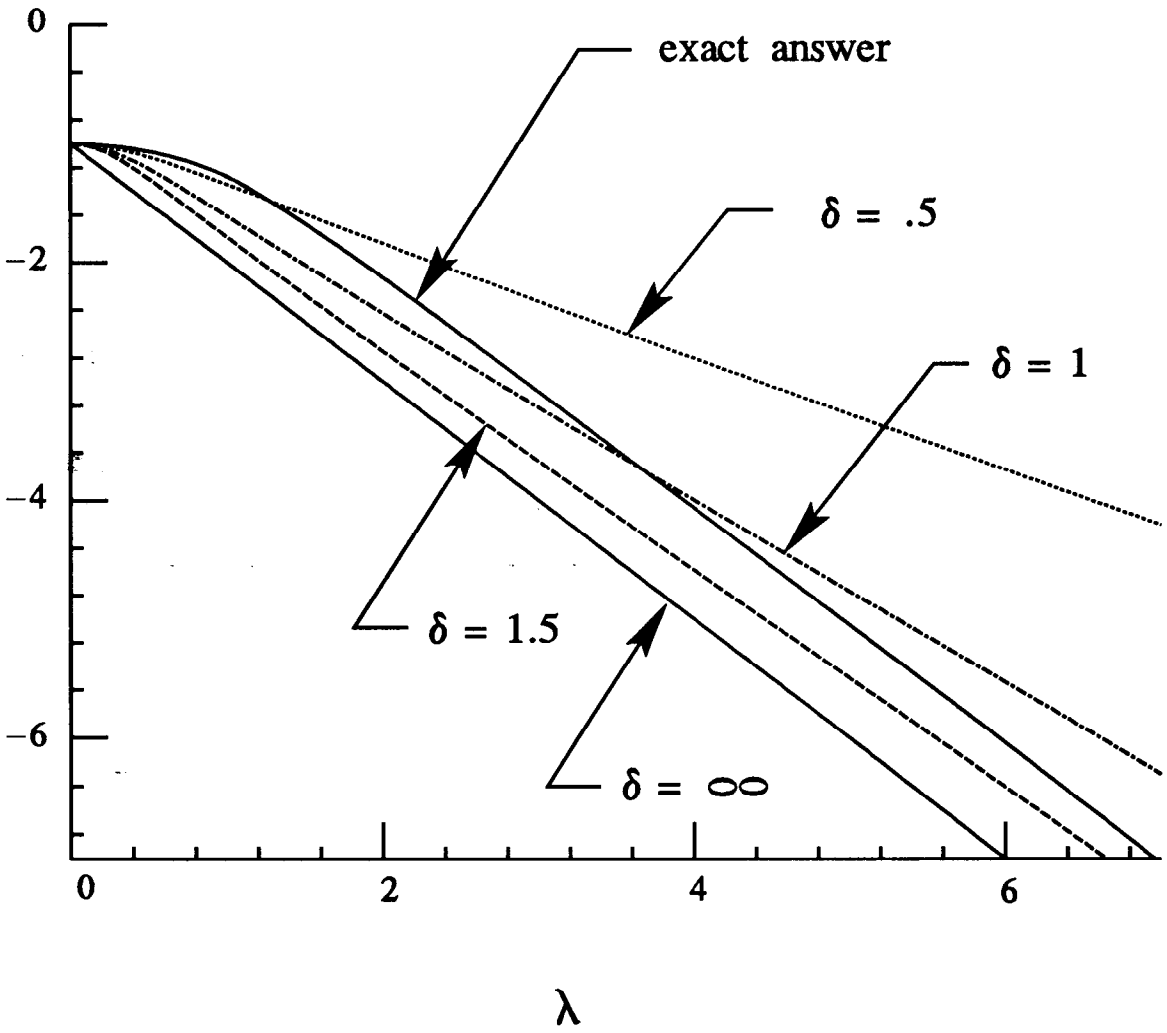

Fig. 4

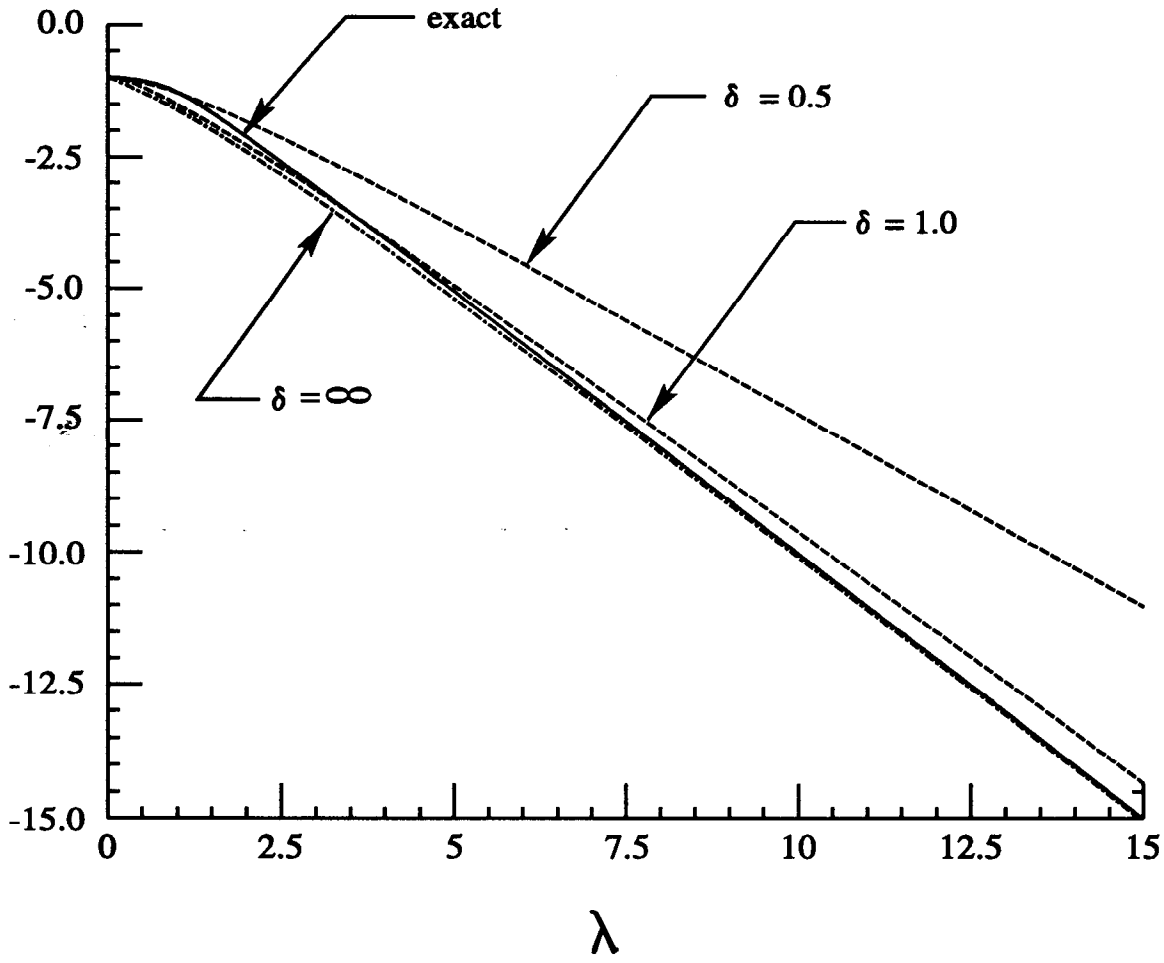

Fig. 5