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Operator Renormalization Group*

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ABSTRACT

We introduce a novel operator renormalization group method. This is a new and more powerful variant of the t -expansion combining that method with the real space renormalization group approach. The aim is to extract infinite volume physics at $t \rightarrow \infty$ from calculations of only a few powers of t . Good results are obtained for the 1 + 1 dimensional Ising model. The method readily generalizes to higher dimensional spin theories and to a gauge invariant treatment of gauge theories. These theories will require greater computational power.

1. Introduction

Despite advances in high speed computing, accurately extracting the physics from a lattice theory of gauge fields and fermions remains a problem. One hope is that Monte Carlo calculations based upon improved algorithms and run on more powerful machines will eventually remedy this situation. It is, however, important to ask if there are other ways to obtain information which can complement the insight one obtains from numerical simulations. In this paper we present a method for dealing with Hamiltonian systems which is analytic in nature, and which uses the computer primarily as a device for doing algebra. The technique we will discuss is, in its conception, a variational calculation; in execution, it combines the Hamiltonian real-space renormalization group with a scheme for systematically improving a variational calculation to any desired level of accuracy. While the Hamiltonian real-space renormalization group^(1,2) has been discussed in the literature, and the improvement technique has been presented under the name *t*-expansion,³ the development of a conceptual and computational framework for combining these ideas is new. In the process of presenting such a framework we broaden our understanding of the original *t*-expansion and clarify the relation between the new Hamiltonian renormalization group and the Euclidean renormalization group of Kadanoff and Wilson.⁴ We also develop a new way of extracting physical quantities which makes no use of the Padé approximation used in earlier versions of the *t*-expansion.

1. TRUNCATION ALGORITHMS

The Hamiltonian real-space renormalization group method is a variational calculation. To see this, consider a wavefunction which depends upon n parameters, $|\alpha_1, \dots, \alpha_n\rangle$, and compute the expectation value

$$E(\alpha_1, \dots, \alpha_n) = \frac{\langle \alpha_1, \dots, \alpha_n | H | \alpha_1, \dots, \alpha_n \rangle}{\langle \alpha_1, \dots, \alpha_n | \alpha_1, \dots, \alpha_n \rangle} \quad (1)$$

One can minimize over the α 's in order to find the best bound on the ground state energy which can be obtained using a this class of trial wavefunctions. One way to choose a trial wavefunction is to consider a state of the form

$$|\alpha_1, \dots, \alpha_n\rangle = \sum_i \alpha_i |i\rangle \quad (2)$$

where the states $|i\rangle$ are some subset of a complete set of states. The problem of minimizing the function $E(\alpha_1, \dots, \alpha_n)$ is equivalent to finding the lowest eigenstate of the *truncated* Hamiltonian

$$[[H]] = PHP^\dagger \quad (3)$$

where P is the projection operator

$$P = \sum_i |i\rangle \langle i| \quad (4)$$

This rewriting of the variational problem as the problem of diagonalizing a new Hamiltonian acting on a reduced number of degrees of freedom is the heart of the Hamiltonian real-space renormalization group procedure. One starts with

a complete set of states and then eliminates certain linear combinations of the initial states in a sequence of steps. The choice of which states to eliminate at each step is referred to as the *renormalization group algorithm* and the mapping from the Hamiltonian at step n to a new one at step $n + 1$ is the *renormalization group transformation*. If one parametrizes the states which one retains these parameters can be thought of as the $\alpha_1, \dots, \alpha_n$ appearing in the generic variational wavefunction.

1. IMPROVING A VARIATIONAL CALCULATION

Historically there has been no systematic way to improve upon a variational calculation. The trial wavefunction is typically not the lowest eigenstate of any simply diagonalizable Hamiltonian; thus, one has no general procedure for setting up a perturbation expansion about the trial wavefunction which actually minimizes the expectation value of the Hamiltonian. One possible solution to this problem is the t -expansion. The physical concept behind the t -expansion is the observation³ that the quantity

$$E(t) = \frac{\langle \psi | H e^{-Ht} | \psi \rangle}{\langle \psi | e^{-Ht} | \psi \rangle} \quad (5)$$

converges to the ground state energy as $t \rightarrow \infty$ for almost any wavefunction $|\psi\rangle$. To exploit this fact in practice, one calculates a finite number of terms in the Taylor-series expansion of (5) and then extrapolates this series to obtain $t \rightarrow \infty$ limit.

There are two difficulties inherent in the t -expansion. The first is the algebraic problem of computing high order terms in the expansion, since there are many such terms. The second is the problem of extrapolating the power series so

obtained to $t \rightarrow \infty$. Our approach to the first problem is to use a computer to carry out the analytic calculation of the coefficients of the power series for $E(t)$. To handle the second question we introduce a new technique for reconstructing the large t behavior of physical quantities based upon known analytic properties of the function being computed. This extrapolation method yields much greater accuracy for fewer terms in the series. In the past we used Padé approximants to carry out this extrapolation, however the arbitrariness of that procedure for low powers of t led us to abandon that approach.

1. COMBINED METHOD

In past applications of the t -expansion the state $|\psi\rangle$ was chosen to be either the strong coupling ground state, for the case of a lattice gauge theory, or a mean-field state, for the case of a quantum spin model. For those values of the coupling constant for which states of this form provide good approximations to the true ground state it is no surprise that one obtains good results for relatively few terms in the expansion; however, as we move further away from this region of couplings, convergence slows down. One expects the t -expansion to converge much faster if one starts with a trial state which has a large overlap with the true vacuum state. For this reason we have combined the t -expansion with the Hamiltonian real-space renormalization group procedure in order to construct a better wavefunction. We use the freedom in the choice of the parameters of the renormalization group transformation to improve the accuracy of the calculation.

This paper reports on the application of this technique to the 1+1-dimensional Ising model; the results show that the expectation that this procedure will produce better results for fewer terms in the expansion is indeed correct. In addition,

by using the renormalization group, or block-spin, procedure, one eventually arrives at a simple effective Hamiltonian which describes not only the ground state, but also the low-lying excited states of the original system. We exploit this fact in the case of the Ising model. Clearly, the Ising model is of interest only as a simple system for testing out this new method.

1. OUTLINE

Section 2 presents a brief derivation of the new operator t -expansion. This derivation is considerably simpler than the one presented in earlier papers and generalizes the results obtained in those papers in a way which allows us to use them with variational wavefunctions derived from a series of renormalization group transformations. The explicit application of the operator t -expansion formula to the case of the 1+1-Ising model is described in Section 3 and in the Appendix. In Section 4 we discuss a method for reconstructing the $t \rightarrow \infty$ behavior of physical quantities from a finite power series in t . In section 5 we present the results obtained by applying this method to the 1+1-Ising model. Finally, in Section 6, we discuss the outlook for applying these methods to theories of greater interest to particle and condensed matter physics. In particular we discuss the generalization of this approach to theories in higher dimensions and to those which involve gauge fields and fermions. We will show that by combining the operator t -expansion and real-space renormalization group methods one obtains, for the first time, a way of carrying out truly gauge invariant Hamiltonian renormalization group studies of this class of theories.

2. Operator t -Expansion

The quantity, $E(t)$, which appears in equation (1) is the the expectation value of the Hamiltonian in a specific state. Taking the expectation value reduces our minimization problem to studying the properties of an ordinary function of several variables. $E(t)$ is propotional to the volume and in the limit $t \rightarrow \infty$ becomes the true groundstate energy. The simplest way of deriving the t -expansion for $E(t)$ is to observe that

$$E(t) = -\frac{d}{dt} \ln Z(t) \tag{1}$$

where

$$Z(t) = \langle \psi | e^{-tH} | \psi \rangle. \tag{2}$$

If we define $A(t)$ to be

$$\begin{aligned} A(t) &= \ln Z(t) \\ &= \ln \left[1 + \sum_{n=1}^{\infty} \left\langle \psi \left| \frac{(-tH)^n}{n!} \right| \psi \right\rangle \right] \end{aligned} \tag{3}$$

then $E(t)$ is obtained by differentiating $A(t)$ with respect to t ; To obtain a t -expansion for expectation values of other operators, O , one studies

$$O(t) = -\lim_{t \rightarrow \infty} \frac{\partial^2}{\partial t \partial j} \ln Z(t, j) |_{j=0}. \tag{4}$$

where $Z(t, j)$ is defined to be

$$Z(t, j) = \left\langle \psi \left| e^{-t(H+jO)} \right| \psi \right\rangle \tag{5}$$

Let us now consider a partial reduction of the problem; wherein we study the truncation of e^{-tH} to a subspace of the original Hilbert space. This is the

problem which arises naturally when we attempt to apply the ideas of the t -expansion to a wavefunction which is constructed by performing a sequence of renormalization group transformations. In what follows the truncation of an operator to a subspace of the original Hilbert space will be indicated by enclosing them in double brackets, i.e., $[[\]]$. For example we define an *operator* $A(t)$, which acts upon the subspace spanned by the retained states by

$$e^{-A(t)} = [[e^{-Ht}]]. \quad (6)$$

The new Hamiltonian acting on this subspace is defined to be

$$\mathcal{H}(t) = \frac{\partial}{\partial t} A(t). \quad (7)$$

The formula for the t -expansion of the energy function $E(t)$ is equivalent to a linked cluster expansion³ — thus it corresponds to a summation over connected diagrams. This follows from the fact that the logarithm in Eq. (3) is an extensive function of the volume. (The definition of connected depends upon the wavefunction ψ , but in any wavefunction generated by a block-spin algorithm it will have a well-defined meaning.) Disconnected contributions always cancel in Eq.(4) and likewise in the operators $A(t)$ and $\mathcal{H}(t)$ defined above. Thus, the logarithm of Eq. (6) will define $A(t)$ as a sum of connected diagrams. This point is explained in the Appendix within the context of the block-spin method described in the next section.

3. Real-Space Renormalization Group

The real-space renormalization group (block-spin) method develops a wavefunction by successive thinning of degrees of freedom. The lattice is divided into non-overlapping blocks of sites. The Hilbert space is then thinned by a truncation to the same subset of states on each block of sites. The definition of this subset involves one or two parameters. An algorithm for fixing these parameters is needed to fully define the block-spin procedure. This algorithm is usually based on minimizing some variational estimate of the ground-state energy.

For a 1+1 dimensional spin- $\frac{1}{2}$ theory² a simple choice is to divide the space into two-site blocks. On each block one then retains only two states, for example

$$|\uparrow\rangle = \cos\theta |\uparrow\uparrow\rangle + \sin\theta |\downarrow\downarrow\rangle \quad \text{and} \quad |\downarrow\rangle = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \quad (1)$$

which belong to two different sectors of Hilbert space within the block. The angle θ is chosen variationally. One can readily calculate the result of this truncation for all possible operators on the block. For example

$$[[1 \cdot \sigma_x]] = [[\sigma_x \cdot 1]] = \frac{\cos\theta + \sin\theta}{\sqrt{2}} \sigma_x \quad (2)$$

where, on the right hand side, σ_x denotes an operator in the basis of states (1). Table 1 contains the results of truncations for all possible pairs of operators.

In the conventional block-spin formulation² one generates consecutive Hamiltonians by the definition

$$\mathcal{H}_{n+1} = [[\mathcal{H}_n]] \quad (3)$$

where \mathcal{H}_{n+1} acts in the restricted basis (1), and $[[\]]$ denotes the truncation to

this basis on every two site block. The Ising model defined by

$$H = - \sum_i [\sigma_z(i) + \lambda \sigma_x(i) \sigma_x(i+1)] \quad (4)$$

generates consecutive effective Hamiltonians of the form

$$\mathcal{H}_n = \sum_i [c_n^I + c_n^z \sigma_z(i) + c_n^{zx} \sigma_x(i) \sigma_x(i+1)]. \quad (5)$$

Given a starting Hamiltonian $\mathcal{H}_0 = H$ one can perform successive truncations to define \mathcal{H}_n . The choice of angle θ_n can be made at each step by minimizing the mean-field estimate of the ground state energy density in the resulting truncated theory. Each site of the truncated theory after n truncations represents 2^n sites of the original lattice. The procedure thus gives a sequence of energy estimates which converges to a fixed result as the recursion proceeds until either c_n^z or c_n^{zx} has become zero and the other has reached a finite value. At this point \mathcal{H}_n can be trivially diagonalized and one can read off the energy density and the mass gap. Further recursions do not alter these results.

We introduce a new mapping $\mathcal{H}_n \rightarrow \mathcal{H}_{n+1}$ by considering $\exp(-Ht)$ as the basic quantity to be iterated. We define $A_0 = Ht$ and the recursion procedure

$$A_{n+1}(t) = - \ln[e^{-A_n(t)}] \quad (6)$$

where A_n is an effective action, from which one may obtain an effective Hamiltonian by

$$\mathcal{H}_n = \frac{\partial}{\partial t} A_n. \quad (7)$$

Equation (6) produces an operator cumulant expansion for A_{n+1} as shown in the Appendix. In general A_n is an infinite power series in t involving an infinite

number of operators. However, the cumulant expansion guarantees that the only non-vanishing terms arise from connected products of the operators in A_{n-1} . Hence, if one calculates the terms in A_n only up to some maximum power T of t , one obtains only a finite set of operators throughout the calculation. Successively higher values of T provide improved approximations to eq. (6). For $T = 1$ this procedure reproduces the previous mapping given by eq. (3), and one obtains for the Ising problem a generalized Hamiltonian of the type of eq. (5). For higher T further operators appear in A_n and hence in \mathcal{H}_n . For example at $T = 2$ the generic form of A_n is given by

$$A_n = \sum_i [a_n^I + a_n^z \sigma_z(i) + a_n^{xz} \sigma_x(i) \sigma_x(i+1) + a_n^{zzx} \sigma_x(i) \sigma_z(i+1) \sigma_x(i+2)] \quad (8)$$

where the coefficients obey the recursion relations

$$a_{n+1}^I = 2a_n + \cos 2\theta_n a_n^z + \frac{1}{2}(1 + \sin 2\theta_n) a_n^{xx} - \sin^2 2\theta_n (a_n^z)^2 + \frac{1}{2} \sin 4\theta_n a_n^z a_n^{xx} \\ + \frac{1}{8}(-5 + 2 \sin 2\theta_n + 3 \sin^2 2\theta_n) (a_n^{xx})^2$$

$$a_{n+1}^z = \cos 2\theta_n a_n^z - \frac{1}{2}(1 - \sin 2\theta_n) a_n^{xx} - \sin^2 2\theta_n (a_n^z)^2 \\ + \frac{1}{4} \sin 4\theta_n a_n^z a_n^{xx} - \frac{1}{4} \cos^2 2\theta_n (a_n^{xx})^2$$

$$a_{n+1}^{xxx} = \frac{1}{4} \cos^2 2\theta_n (a_n^{xx})^2$$

$$a_{n+1}^{xx} = \frac{1}{2}(1 + \sin 2\theta_n) a_n^{xx} + \cos 2\theta_n a_n^{zzx} + \frac{1}{2} \sin 4\theta_n a_n^{xx} a_n^z - \frac{1}{2} \cos^2 2\theta_n (a_n^{xx})^2$$

Here θ_n stands for the angle used in the definition of states in eq. (1) for this truncation step. The coefficients of the corresponding operators in \mathcal{H}_n are given by

$$c_n = \frac{\partial}{\partial t} a_n.$$

The coefficients a_n^I , a_n^z , and a_n^{xx} contain terms that are both linear and quadratic in t whereas a_n^{xxx} is purely quadratic. Any higher t -powers are disregarded in the $T = 2$ approximation.

For $T = 3$ one has to allow for two additional operators of the form $xzxx$ and yy , leading to a more complicated set of recursion relations. The number of operators increases considerably as T is increased, thus this formulation of the renormalization-group procedure generates terms in a much bigger space of operators than the conventional block-spin method. We have developed a computer program which carries out the truncation calculation analytically. This generates the recursion relations which depend on the various parameters of the starting $\chi_0 = H$ as well as the values of θ_n , the wavefunction parameters which have to be chosen for each successive truncation. The choice of these parameters is guided by the ansatz for Z described in the next section.

4. Parametrizing Z as a Sum of Exponential Factors

When the t -expansion is calculated to finite order t^T and the renormalization group procedure is carried out to n iterations, the connected diagrams have a range limited by

$$V_{eff} = 2^n(T + 1). \quad (1)$$

Thus, to this order, our calculation also gives the correct $Z_L(t)$ for the theory defined on a lattice of L sites with periodic boundary conditions provided $L > V_{eff}$. A bound on the ground state energy of the finite-volume theory can be

derived exploiting the known analytic behavior

$$Z_L(t) = \sum_m \alpha_m^L e^{-\mu_m^L t} \quad (2)$$

which follows trivially from the definition of the finite quantum-mechanical system, where the μ_m^L are the eigenvalues of the finite-volume Hamiltonian. By adding a large enough constant to H one can ensure that all eigenvalues are positive, as are the weights α_m^L . The lowest eigenvalue μ_1^L is an upper bound on the vacuum energy of the finite-volume theory. Since we have only a finite t -series we cannot retrieve all the rich structure of Eq. (2), we can however obtain an upper bound on μ_1^L .

Consider the approximation

$$Z_L(t) \approx \sum_{m=1}^P \beta_m^L e^{-\nu_m^L t}. \quad (3)$$

For $2P = T + 1$ we can determine uniquely all parameters by matching the first $2P$ terms of the Taylor expansion of the right hand side with the t -expansion for Z . Working with the Laplace transform of Z which gives the resolvent operator

$$R_L(s) = \left\langle \psi^L \left| \frac{1}{s - H} \right| \psi^L \right\rangle \quad (4)$$

Bessis and Villani⁵ proved that the true eigenvalues are bounded from above by the approximate ones

$$\nu_m^L > \mu_m^L \quad m = 1, \dots, P \quad (5)$$

and furthermore that the bounds decrease monotonically as P increases. Thus the smallest of the ν_m^L in (3) produces a strict bound on the energy density of the finite volume theory.

This method can be applied to the t -expansion about a mean field state (or strong coupling eigenstate for a gauge theory) and gives considerable improvement over the Padé approximants for the same series.

The infinite volume theory can be approximated by the finite volume one in the following way

$$Z_{NL}(t) = Z_L(t)^N + O(t^L). \quad (6)$$

Thus we can use the approximation

$$Z_V(t) \approx \left[\sum_{m=1}^P \beta_m^L e^{-\nu_m^L t} \right]^N \quad (7)$$

where $N = V/L$ diverges with the volume V . This gives us an estimate for the vacuum energy density

$$\epsilon = \frac{\nu_1}{L}. \quad (8)$$

Equation (7) may be interpreted as a mapping of our problem onto a non-interacting lattice theory with P levels per L -site block. Since there are originally 2^L states on L sites it is clear that approximating the spectrum by a set of P independent eigenvalues will work better for smaller L . This result was found empirically by Banks and Zaks⁶ in their application of the resolvent operator method to lattice theories. The minimum L value for which there is guaranteed to be a fit of the form (7) with positive weights and eigenvalues is $L = V_{eff}$.

We could now proceed in the following way: after the n -th truncation choose a trial function

$$\cos \phi_{n+1} (\cos \theta_{n+1} |\uparrow\uparrow\rangle + \sin \theta_{n+1} |\downarrow\downarrow\rangle) + \sin \phi_{n+1} \left(\frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \right) \quad (9)$$

and use it for evaluating

$$Z_L(t) = \langle \psi^L | e^{-A_n(t)} | \psi^L \rangle \quad (10)$$

with $L = V_{eff}$. Vary the angles until the minimal ν_1 is obtained. Then choose the ket multiplied by $\cos \phi_{n+1}$ as the new $|\uparrow\rangle_{n+1}$ and the other combination as $|\downarrow\rangle_{n+1}$. These form the basis for the next truncation step. Using this procedure we find that the energy estimate decreases in the first few truncations then goes through a minimum and increases as one continues to iterate the procedure. The reason is that as V_{eff} increases the lowest exponent dominates in Eqs. (3) and (7) and the method loses its ability to discern the correct structure.

One major advantage of the t -expansion formulation is that one can avoid all volume dependence and derive results which are directly relevant to the infinite lattice. The problem one faces is that of reconstruction of the series. Padé approximant techniques are general-purpose tools which may be applied to the energy as well as to other operators. An alternative procedure which we find more stable and which gives better numerical results is to use, at every level of the recursion procedure, an exponential ansatz of the type (7), but with fixed rather than increasing L . If we choose $L = 2(T + 1)$ then in the first truncation step there are no connected diagrams of range greater than L , and thus we are guaranteed positive weights and eigenvalues. At subsequent truncation steps much information about the original theory has accumulated in the unit operator in $A(t)$. When this dominates the fit no large error is made and the fitted weights and eigenvalues remain positive, even though there now exist a few connected diagrams with range greater than L . We require that the parameters obtained this way for Eq. (3) obey the positivity conditions necessary for the interpretation

of this method as a mapping onto an equivalent free Hamiltonian system. In fact we find for the Ising model that a procedure where the variational angles are chosen by minimizing the energy density from this fixed- L fit always satisfies the positivity test and gives extremely good results, provided L is chosen large enough. Below the phase transition the minimum value of L , $L = 2(T + 1)$ is satisfactory. Above the phase transition the recoupling terms in \mathcal{K} are not iterating away and thus at large values of λ they can still cause significant wrap-around contributions after a few iterations. At large enough λ this introduces instabilities into the fitting procedure and eventually gives results which violate the positivity requirements. We find that these problems are avoided by working with a slightly larger value of L , at the cost of a small decrease in accuracy. The investigation of the dependence of the final results on the value of L used in the reconstruction, and the determination of a description to use for choosing L as a function of the coupling constant, has not yet been made.

5. Results of Calculations

The calculation described in the preceding sections produces a very accurate estimate of the ground state energy density using only a few powers of t . In this section we display our results and compare them with other calculations. Figure 1(a) shows the energy density as a function of λ for $L = 9$ as extracted from fits to the t^1 , t^3 , and t^5 series about the state chosen by minimizing the t^5 energy estimate. In this and subsequent figures we show results of the $L = 9$ calculation as a conservative choice. The $L = 6$ reconstructions are well behaved up to about $\lambda = 1.3$, however the $L = 9$ reconstructions are well behaved to much larger values of λ . Figure 1(b) shows the error in the energy estimate extracted

from the t^5 calculations for both $L = 6$ and $L = 9$; one clearly sees that some accuracy is lost by going to the larger L value. For comparison we also show here the result obtained from a t^7 expansion about a mean field state using the dPadé³ method to reconstruct the $t \rightarrow \infty$ value of the energy. We see that the improvement given by the new procedure is substantial, the lower order block-spin calculation is better than the higher order mean-field result, a fact that is also reflected in the value of the critical point. Figure 2 shows the quantity $\partial\epsilon/\partial\lambda$ and again compares the $L = 9$ calculations with the exact results. In Figs. 3(a) and (b) we present $\partial^2\epsilon/\partial\lambda^2$ as given by this Operator Renormalisation Group (ORG) calculation, compared to the exact result. We see the behavior of the exact theory is quite well reproduced by the t^5 calculation except that the critical point is somewhat misplaced. In Table 2 we compare the values of the critical point and the energy density at $\lambda = 1$ obtained with various approximate calculations. The rapid improvement in the location of the critical point is of particular interest since this quantity is not universal and depends upon the details of the specific Hamiltonian.

Because we keep two distinct states per block, we can also make mass gap estimates from this calculation. Below the phase transition the effective action iterates to a form

$$A(t) = a_u^n(t) + a_z^n(t)\sigma_z \quad (1)$$

with all other operator coefficients vanishing like $(1/2^n)$. We can then readily diagonalize the resulting theory after a sufficient number n of interactions. On a volume $V = 2^n$, i.e. one block of sites, the two states $|\uparrow\rangle_n$ and $|\downarrow\rangle_n$ belong to distinct sectors of the Hilbert space of the starting Hamiltonian \mathcal{H}_0 . The state

$|\uparrow\rangle_n$ contains only terms with even numbers of spins up and $|\downarrow\rangle_n$ has only odd numbers of spins up and \mathcal{H}_0 only flips spins in pairs. Hence we can evaluate

$$Z_{V=2^n}^\uparrow = {}_n \langle \uparrow | e^{-\mathcal{H}_0 t} | \uparrow \rangle_n \quad (2)$$

and

$$Z_{V=2^n}^\downarrow = {}_n \langle \downarrow | e^{-\mathcal{H}_0 t} | \downarrow \rangle_n . \quad (3)$$

For each of these we make an ansatz of the form of Eq.(7) with $N = V/L$ and $L = 9$ as in the energy density calculation described previously. The mass gap is then given by

$$m = \frac{V}{L} (\nu_1(\downarrow) - \nu_1(\uparrow)) \quad (4)$$

where $\nu_1(\downarrow)$ is the lowest exponent for the state $|\downarrow\rangle_n$ and similarly $\nu_1(\uparrow)$ for the state $|\uparrow\rangle_n$. This gives an estimate which stabilizes after sufficiently many iterations, since the corrections vanish as $(1/2^n)$.

To see that this estimate is also valid for the infinite volume case, consider K blocks of sites. If all blocks are in the state $|\uparrow\rangle_n$ then we have the ground state of the original theory and

$$Z_{V=K \cdot 2^n} = \left\langle \prod_{i=1}^K (\uparrow_n)_i \middle| e^{-\mathcal{H}_0 t} \middle| \prod_{i=1}^K (\uparrow_n)_i \right\rangle = \left(Z_{V=2^n}^{(\uparrow)} \right)^K \quad (5)$$

whereas the first excited state is given by $(K - 1)$ blocks in the state $|\uparrow\rangle_n$ and any one block in the state $|\downarrow\rangle_n$. For this state

$$Z_{V=K \cdot 2^n} = \left[Z_{V=2^n}^{(\uparrow)} \right]^{K-1} \left[Z_{V=2^n}^{(\downarrow)} \right] \quad (6)$$

and the mass gap given by (5) and (6) is exactly that of Eq. (4).

Above the phase transition the iteration converges to

$$A(t) = a_u^n(t) + a_{xx}^n(t)\sigma_x\sigma_x \quad (7)$$

All other coefficients iterate to zero. Now there are clearly two degenerate ground states on a block of $V = 2^n$ sites; namely,

$$\begin{aligned} |\psi_R^n\rangle &= \frac{1}{\sqrt{2}} (|\uparrow\rangle_n + |\downarrow\rangle_n) \\ |\psi_L^n\rangle &= \frac{1}{\sqrt{2}} (|\uparrow\rangle_n - |\downarrow\rangle_n) \end{aligned} \quad (8)$$

On a volume $V = 2^{n+1}$ we can estimate the gap to the single kink state by calculating

$$Z_{V=2^{n+1}}^{RR} = \left\langle \psi_R^n \psi_R^n \left| e^{-\lambda_0 t} \right| \psi_R^n \psi_R^n \right\rangle \quad (9)$$

and

$$Z_{V=2^{n+1}}^{RL} = \left\langle \psi_R^n \psi_L^n \left| e^{-\lambda_0 t} \right| \psi_R^n \psi_L^n \right\rangle. \quad (10)$$

Again we use an ansatz of the form of Eq. (7) with $L = 9$.

The mass of the kink state is again given by (4). The results for the mass gap are shown in Fig. 4. These are calculated from the ($t^5, L = 9$) ORG calculation. The set of mass values corresponding to the points denoted by circles in Fig.4 are obtained using the full \mathcal{H}_n . The second set of values, indicated by squares, are calculated by dropping the terms in \mathcal{H}_n that are proportional to the unit operator. These terms should contribute equally to the energy of each of the two states. Since these terms include some higher powers of t the two mass estimates are not identical. The region where the two methods agree is where we expect

the mass estimate to be most reliable, and indeed this turns out to be the case for the Ising model.

We see that the results for the mass obtained below the phase transition are much better than results obtained above the phase transition. This difference is built into our choice of states in the recursion calculation. Below the phase transition, even our restricted Hilbert space includes the lowest excitation, a single flipped spin in a zero momentum plane wave on the original lattice. Because we keep both degenerate ground states above the phase transition we can construct kink-like excitations, but only with the kink at a block boundary, we cannot fully reconstruct a kink state with zero momentum on the original lattice. There are clearly ways to improve this calculation above the phase transition, one could even choose a block spin algorithm which is explicitly self-dual. Since the purpose of this paper is to show the efficacy of the new calculation method, and not to utilize our knowledge of the Ising model to the fullest, we think it is preferable to show results obtained using a single choice of block spin algorithm and the same value of L , for all values of the coupling constant λ . It is clear, however, that in future applications of this method it would be useful to explore the freedom to vary the truncation algorithm and the choice of L with coupling constant.

6. Outlook

As the results of the previous section show the combination of t -expansion and block-spin methods is considerably more powerful than either approach used separately. In this section we discuss the application of this technique to more interesting theories. The method can readily be used for higher dimensional spin theories. Furthermore, if one keeps only a number of *gauge invariant* states per block, a gauge theory is mapped, in a single block-spin step, into a spin theory. Thus, the method allows us to use block-spin ideas in a gauge theory while at the same time maintaining full gauge-invariance at every step. Let us discuss these points in some further detail.

In any block spin calculation there are two choices which must be made at the start of the calculation

- (i) How will the lattice be divided into blocks.
- (ii) How many states per block will be retained.

In general it is desirable to choose blocks of p sites so that the new lattice formed by treating the center of each block as a new site has the same structure as the original lattices. On a regular d -dimensional cubic lattice blocks of $p = 2^d$ or $p = 3^d$ sites have this property and either can be used.

If one retains N states per block then the generic recursion is a truncation from p^N states to N states chosen from these p^N with some set of variational parameters. The accuracy of the calculation at a given maximum power of t will depend on how these states are chosen—the variational parameters should allow one to span the lowest lying states of the generic Hamiltonian restricted to a single block for all choices of Hamiltonian parameters.

If the starting theory is not a spin- S theory ($N = 2S + 1$) then the first block spin step will be different from the generic recursion step; i.e., it will map the initial theory into a theory with N states per site. For example when the starting theory is a pure gauge theory there are originally only link operators and there is an infinite spectrum of link excitations. A gauge invariant prescription can be obtained by choosing to keep only states which can be created from the strong coupling ground state by acting with any superposition of those plaquette operators which act only on plaquettes totally within the block of sites. Any set of N orthogonal states within this subset of the Hilbert space of a single block is an acceptable prescription. It is preferable to use states which belong to different sectors of the single block Hilbert space, thus representing excitations with different quantum numbers. The variational parameters will appear as the relative weightings of various strong coupling eigenstates in the definition of the N retained states.

For a gauge theory with fermions this prescription can readily be generalized. One again starts from the strong coupling ground state and forms superpositions of states created from this state by the action of gauge invariant operators which are totally contained within the block, either $\text{tr}(UUU^\dagger U^\dagger)$ on internal plaquettes, or $\psi_i^\dagger(\Pi_i^j U)\psi_j$ where the sites and the links addressed by these operators are all internal to a single block.

There is clearly a great deal of arbitrariness in these prescriptions; the essential point to realize is that this does not matter. In principle if one keeps a sufficient number of powers of t in the expansion for all interesting gauge invariant operators in the original theory one can obtain the desired information about the ground state of the original theory with any choice of blocking algorithm. The

only way in which the choice of retained states affects the calculation is in the question of how many powers of t must be calculated to obtain reliable results.

Clearly there are trade-offs which one makes in this kind of calculation. If one keeps more states or introduces more variational parameters in the choice of retained states one can achieve better results from calculating fewer powers of t . However, the work involved in calculating each power of t is greater when there are more states or more variational parameters. The answer as to what procedure works most effectively awaits further study.

In all these generalizations the necessary computing power will be considerably greater than that used in our Ising model example. However, compared with the huge expenditure of computer time in Monte Carlo calculations these methods could be quite efficient. Furthermore, the method is algebraic in nature and should be pursued as an alternative which is complementary to the Monte Carlo method.

APPENDIX

Consider a 1-dimensional lattice. We associate any string of operators on this lattice with the left-most site i addressed by these operators. Thus we can write the effective action as

$$A_n = \sum_{\text{sites } i} a_{nm}(t) O_m(i) . \quad (A.1)$$

The coefficients $a_{nm}(t)$ are polynomials in t . The calculation is carried out keeping terms only up to some power T of t . Then a given starting Hamiltonian ($A_0 = Ht$) generates a finite set of operators O_m which appear in A_n for any n .

We seek to calculate A_{n+1} from A_n using

$$e^{-A_{n+1}} \equiv \llbracket e^{-A_n} \rrbracket. \quad (\text{A.2})$$

When the Hamiltonian contains only finite-range interactions the ground-state energy of the system grows linearly with V . Hence the logarithm of Eq. (A.2) is guaranteed to produce an expression for A_n which can be written in the form of Eq. (A.1). Thus in the expansion

$$\begin{aligned} A_n &= \sum_{k=1}^{\infty} \frac{(-1)^k}{k} \left(\left[\left[\sum_{r=1}^{\infty} \frac{(-A_n)^r}{r!} \right] \right] \right)^k \\ &= \llbracket A_n \rrbracket - \llbracket \frac{A_n^2}{2!} \rrbracket + \frac{1}{2} \llbracket A_n \rrbracket \llbracket A_n \rrbracket \\ &\quad + \llbracket \frac{A_n^3}{3!} \rrbracket - \frac{1}{2} \left(\llbracket \frac{A_n^2}{2!} \rrbracket \llbracket A_n \rrbracket + \llbracket A_n \rrbracket \llbracket \frac{A_n^2}{2!} \rrbracket \right) \\ &\quad - \frac{1}{3} \llbracket A_n \rrbracket \llbracket A_n \rrbracket \llbracket A_n \rrbracket + \dots \end{aligned} \quad (\text{A.3})$$

terms which arise from products of strings of operators on separated regions of the lattice must vanish, that is disconnected graphs must cancel. This was discussed for the t -expansion about a mean-field state in ref. 1. Here we must simply generalize the notion of connectedness for a block-spin calculation. One finds that diagrams cancel unless they correspond to operators acting on a neighboring set of blocks with at least one string of operators overlapping each block boundary.

To show how terms appear in A_n that are not present in the starting $A_0 = Ht$, let us study a term quadratic in A_n of eq. (A.3) which arises from the operators

$\sigma_x(i)\sigma_x(i+1)$ and $\sigma_x(i')\sigma_x(i'+1)$. Let us examine the contribution

$$-\frac{1}{2!} \llbracket \sigma_x(2i+1)\sigma_x(2i+2)\sigma_x(2i+3)\sigma_x(2i+4) \rrbracket$$

$$+\frac{1}{2} \llbracket \sigma_x(2i+1)\sigma_x(2i+2) \rrbracket \llbracket \sigma_x(2i+3)\sigma_x(2i+4) \rrbracket .$$
(A.4)

where the i -th block contains the sites $2i$ and $2i+1$. From Table 1 we can read off the results. The first term gives

$$-\frac{1}{2!} \left(\frac{\cos \theta + \sin \theta}{\sqrt{2}} \right)^4 \sigma_x(i)\mathbf{1}(i+1)\sigma_x(i+2)$$

$$+\frac{1}{2!} \left(\frac{\cos \theta + \sin \theta}{\sqrt{2}} \right)^2 \left(\frac{\cos \theta - \sin \theta}{\sqrt{2}} \right)^2 \sigma_x(i)\sigma_x(i+1)\sigma_x(i+2)$$
(A.5)

while the second term is

$$\frac{1}{2} \left(\frac{\cos \theta + \sin \theta}{\sqrt{2}} \right)^4 \sigma_x(i)\sigma_x(i+1) \cdot \sigma_x(i+1)\sigma_x(i+2) .$$
(A.6)

This cancels the first term in (A.5) and the result is simply

$$\frac{\cos^2 2\theta}{2} \sigma_x(i)\sigma_x(i+1)\sigma_x(i+2) .$$

Thus we see that starting from the operators $\sigma_x\sigma_x$ at order t in A_n we generate the operator $\sigma_x\sigma_x\sigma_x$ at order t^2 in A_{n+1} .

We have written a program in the language C which can perform this calculation systematically up to A^7 or $T = 7$, the principal limitation being computer time. Each successive power of t requires an order of magnitude greater computation time than the preceding power, both because more operators appear in the general form of A_n and because there are clearly many more terms to be computed for $(Ht)^{p+1}$ than for $(Ht)^p$. For the Ising model at $T = 5$ the analytic operator truncation calculation takes only a few IBM 3081 CPU minutes. The $T = 6$ calculation requires a several of hours.

TABLE 1

Truncation of operators in the basis (3.1)

Original operators (on two sites)	Block operator (result of truncation)
$\mathbf{1} \cdot \mathbf{1}$	$\mathbf{1}$
$\left. \begin{array}{l} \mathbf{1} \cdot \sigma_x \\ \sigma_x \cdot \mathbf{1} \end{array} \right\}$	$\frac{\cos \theta + \sin \theta}{\sqrt{2}} \sigma_x$
$\left. \begin{array}{l} \mathbf{1} \cdot \sigma_y \\ \sigma_y \cdot \mathbf{1} \end{array} \right\}$	$\frac{\cos \theta - \sin \theta}{\sqrt{2}} \sigma_y$
$\left. \begin{array}{l} \mathbf{1} \cdot \sigma_z \\ \sigma_z \cdot \mathbf{1} \end{array} \right\}$	$\frac{\cos 2\theta}{2} \mathbf{1} + \frac{\cos 2\theta}{2} \sigma_z$
$\sigma_x \cdot \sigma_x$	$\frac{1 + \sin 2\theta}{2} \mathbf{1} - \frac{1 - \sin 2\theta}{2} \sigma_z$
$\left. \begin{array}{l} \sigma_x \cdot \sigma_y \\ \sigma_y \cdot \sigma_x \end{array} \right\}$	0
$\left. \begin{array}{l} \sigma_x \cdot \sigma_z \\ \sigma_z \cdot \sigma_x \end{array} \right\}$	$\frac{\cos \theta - \sin \theta}{\sqrt{2}} \sigma_x$
$\sigma_y \cdot \sigma_y$	$-\frac{1 - \sin 2\theta}{2} \mathbf{1} + \frac{1 + \sin 2\theta}{2} \sigma_z$
$\left. \begin{array}{l} \sigma_y \cdot \sigma_z \\ \sigma_z \cdot \sigma_y \end{array} \right\}$	$\frac{\cos \theta + \sin \theta}{\sqrt{2}} \sigma_y$
$\sigma_z \cdot \sigma_z$	σ_z

Table 2

Method of Calculation	λ_{crit}
Mean Field	.5
Naive Block-spin	.78
<i>t</i> -expansion about Mean Field, $T = 7$.87
ORG $T = 3$ $L = 4$.89
ORG $T = 5$ $L = 9$.93
ORG $T = 5$ $L = 6$.94

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FIGURE CAPTIONS

- 1) (a) Energy density as a function of λ for the $L = 9$ calculation. Angles have been chosen to minimize the t^5 energy density. (b) Fractional error in the energy density as a function of λ for both the $L = 6$ and $L = 9$ t^5 calculations. For comparison we also show the results of a t^7 expansion about a mean-field state using Padé reconstruction.
- 2) First derivative of the energy density as a function of λ for the $L = 9$ calculation, showing the t^1 , t^3 and t^5 results.
- 3) (a) Second derivative of the energy density as a function of λ for $L = 9$ calculation showing t^1 , t^3 and t^5 results. (b) The t^5 results for $-d^2E/d\lambda^2$ compared to the exact result.
- 4) Mass gap as a function of λ .

TABLE CAPTIONS

- 1: Truncation table.
- 2: Comparison of Calculations.

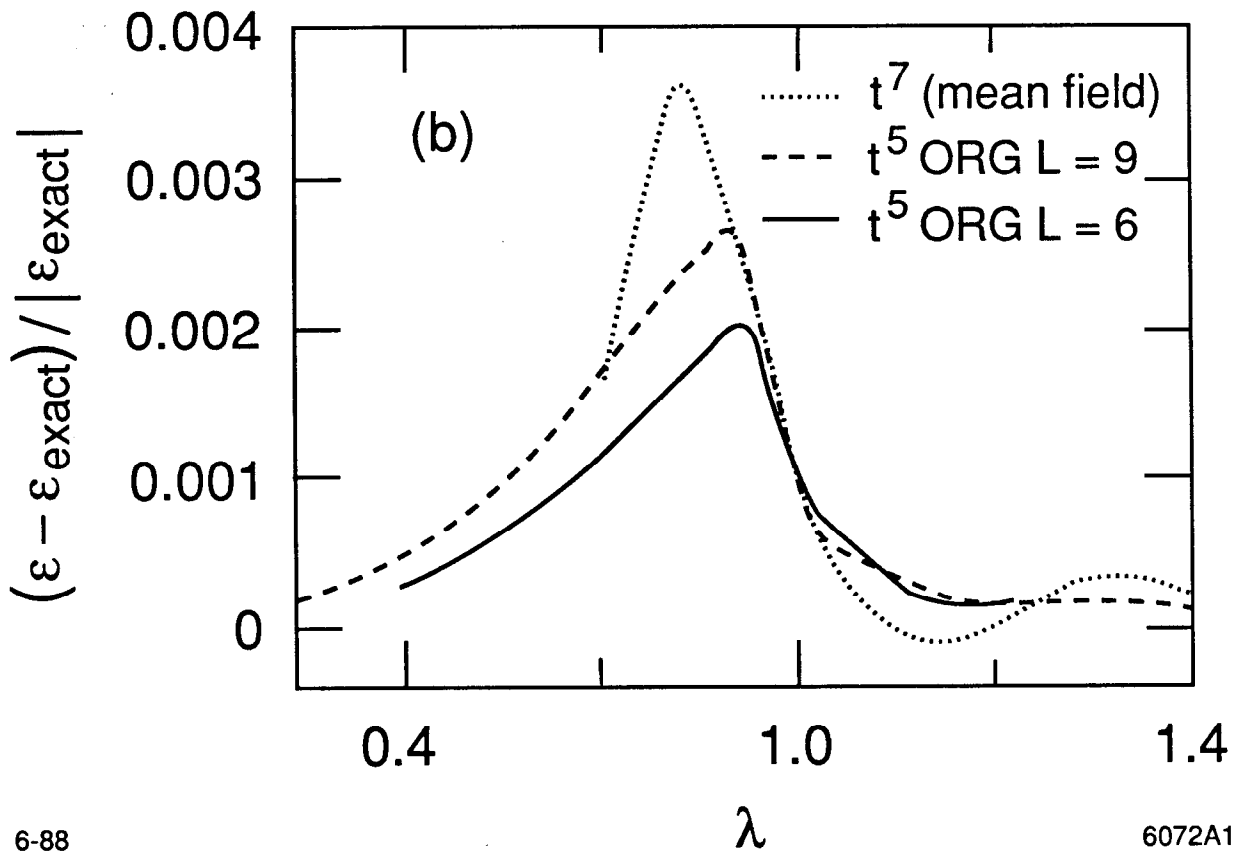
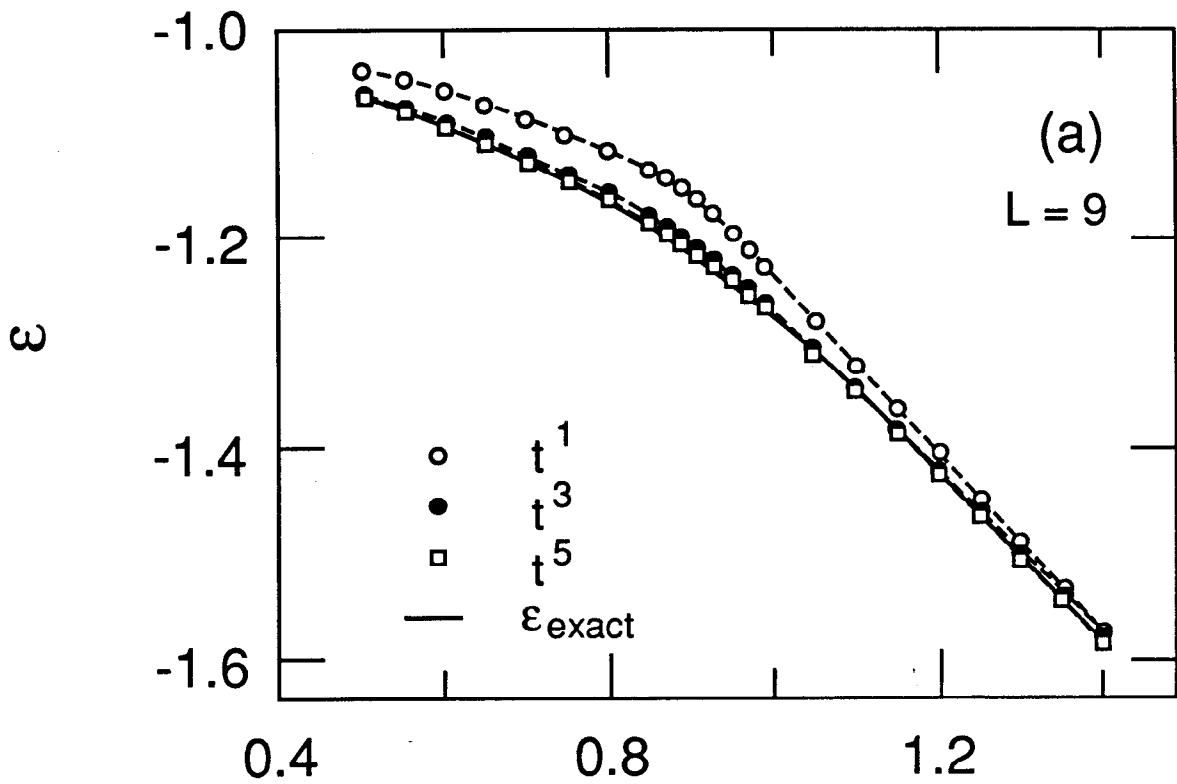


Fig. 1

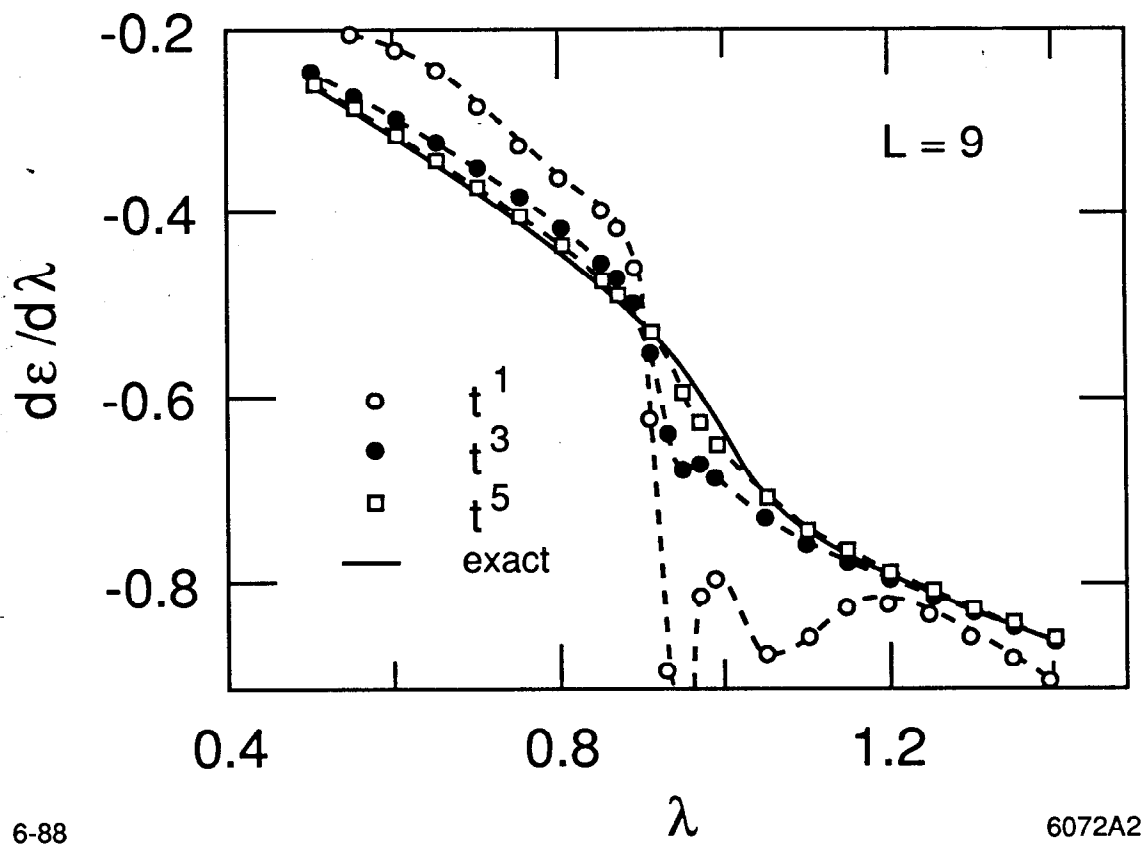


Fig. 2

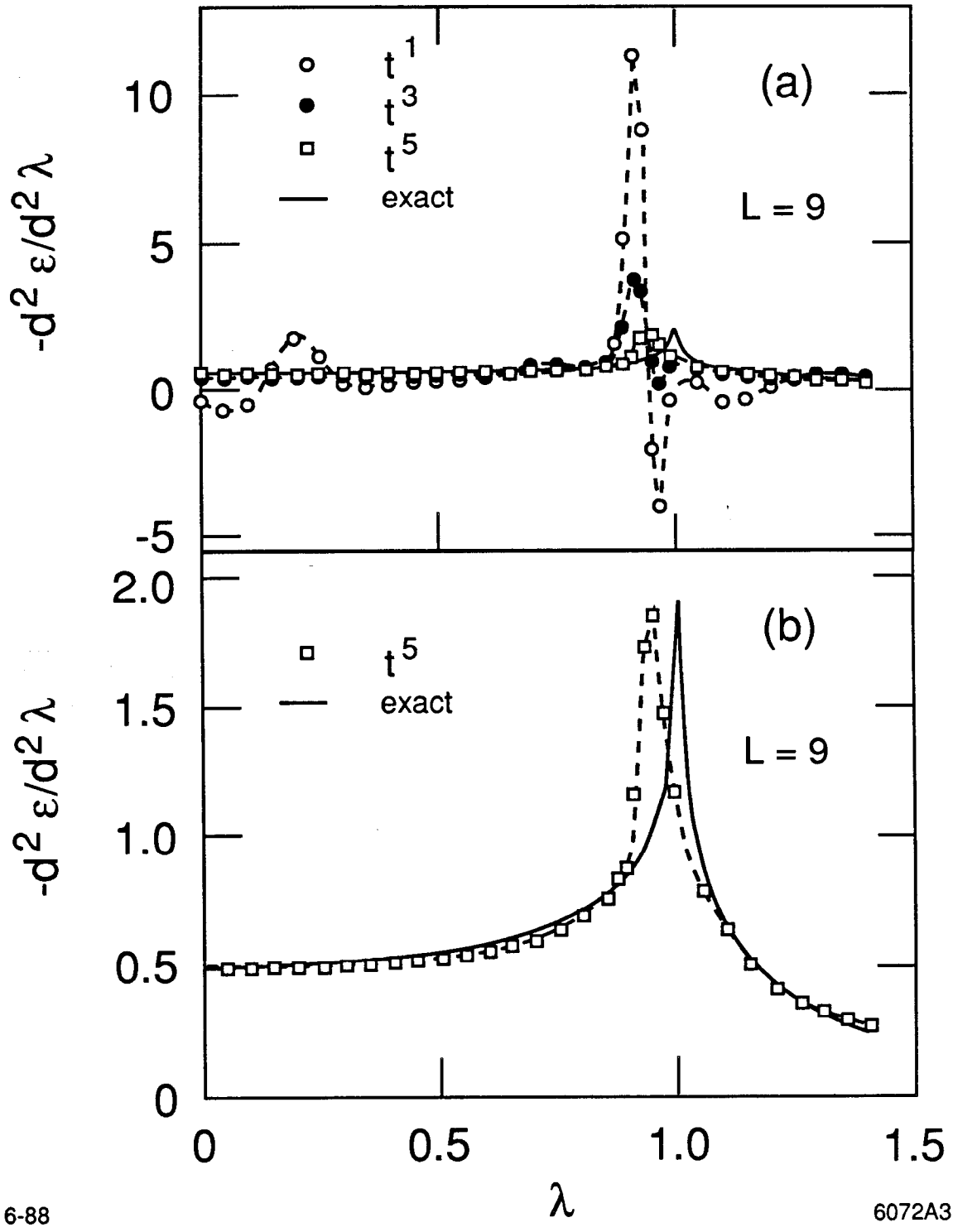
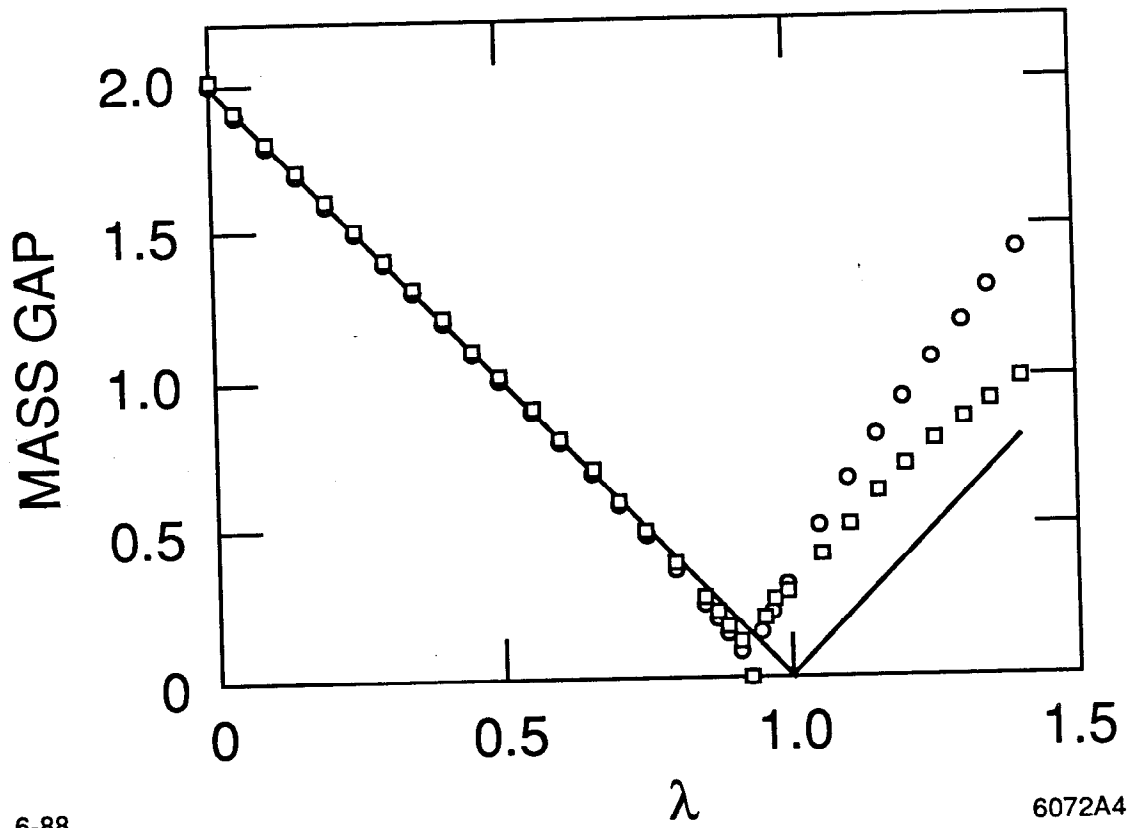


Fig. 3



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Fig. 4