t expansion and the Lipkin model

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(Received 4 January 1988)

We apply the t-expansion method of Horn and Weinstein to the SU(2) soluble model of Lipkin. The method is shown to approximate well both the ground state and the first excited state energies. An extension to a dynamically determined reference state is explored and shown to dramatically improve results for the region of strong coupling.

I. INTRODUCTION

Recently a systematic nonperturbative approach has been developed to calculate ground-state expectation values of arbitrary operators for any Hamiltonian system.[1] It makes use of the operator e^{-tH} which may be considered as the imaginary-time many-body propagator and filters a trial function $|\phi\rangle$ to the exact ground state $|\psi\rangle$ in the limit $t\to\infty$. The method, referred to as the t expansion, systematically improves the results obtained through any variational, or perturbative, calculation and is proving a valuable tool to study field theories in the nonperturbative domain. It has been applied to two dimensional spin systems[1] and to four dimensional nonabelian lattice gauge theories.[2–6]

Since the method is based on a Hamiltonian approach, it is expected to be of great value for the many-body problem as well. To test this is one of the purposes of the present work. Moreover, we want to explore whether known techniques that work well in many-body theory can actually extend the utility of the t expansion method. To accomplish this we examine the validity of the t expansion within a soluble model, the Lipkin model.[7] Exactly soluble models are of great utility as testing grounds for many-body theories of finite fermion systems, not only because they provide exact solutions to be compared with the approximate results but also because their simplicity contributes to the understanding of the approximations involved.

We will show that the t expansion yields an excellent approximation for the ground state and first excited state energies. A particular extension we will consider is the use of a dynamically determined reference state. The particular choice we invoke will be seen to dramatically improve results in the region of strong coupling.

In Sec. II we present a short review of the method, a summary of previous applications and an outline of the present application. In Sec. III we show the results obtained and finally in Sec. IV we draw some conclusions.

II. THE METHOD AND ITS APPLICATIONS

A. Short review of the method

The basic idea of the method is that if one has a starting wave function $|\phi_0\rangle$ that has a nonzero overlap with the true ground state of a quantum system defined by a Hamiltonian H, then the parametrized wave function

$$|\phi_t\rangle=\langle\phi_0|e^{-tH}|\phi_0\rangle^{-1/2}e^{-tH/2}|\phi_0\rangle \tag{2.1}$$

is a better approximation to the exact ground state for any finite value of t. In particular, it is shown[1] that in the limit $t\to\infty$, $|\phi_t\rangle$ converges to the lowest eigenstate of the Hamiltonian. Consequently, the energy expectation value

$$E(t)=\langle\phi_0|He^{-tH}|\phi_0\rangle/\langle\phi_0|e^{-tH}|\phi_0\rangle \tag{2.2}$$

tends to the ground state energy in the same limit. $E(t)$ can be written[1] as a power series in t

$$E(t)=\sum_{m=0}^{\infty}\frac{\langle H^{m+1}\rangle^c}{m!}(-t)^m\ , \tag{2.3}$$

where the connected matrix element of H is defined recursively by

$$\langle H^{m+1}\rangle^c=\langle\phi_0|H^{m+1}|\phi_0\rangle-\sum_{p=0}^{m-1}\begin{bmatrix}m\\p\end{bmatrix}\langle H^{p+1}\rangle^c\langle\phi_0|H^{m-p}|\phi_0\rangle\ . \tag{2.4}$$

In any application one evaluates the series in Eq. (2.3) for a range $0\le n\le L$. The approach proposed in Ref. 1, in order to obtain a good approximation to $E(t)$ over a larger range in t, is to use Padé approximants. They employ two different procedures. The first one is to use the diagonal Padé $[M/M]$ and watch for convergence of the series $M=1,2,3\ldots$. However, this requires going to rather high orders in t which is very difficult in realistic

calculations. Consequently, they turn to the second procedure which considers the derivative of the function $E(t)$ and the Padé approximant to that derivative. Differentiating (2.2) with respect to t one obtains

$$\frac{dE(t)}{dt} = -(\langle \phi_t | H^2 | \phi_t \rangle - \langle \phi_t | H | \phi_t \rangle^2) , \quad (2.5)$$

which means that $dE(t)/dt$ is a function which monotonically increases to zero. Thus, one obtains an upper limit $t_{\max}$ from the value at which the Padé approximant to the derivative becomes positive. Then, one integrates the $[L/L+M]$ Padé approximant for $M \geq 2$ from 0 to $t_{\max}$ to obtain $E(t_{\max})$. This second procedure has been demonstrated to accurately reconstruct $E(t)$ over a larger range in t.

Finally, an extension of the formalism is presented in Ref. 1, called the bistate contraction scheme. It considers two different starting wave functions $|\phi_0\rangle$ and $|\chi_0\rangle$. Then the energy is written as

$$E_{\phi\chi}(t) = -\frac{d(\ln\langle \phi_0 | e^{-tH} | \chi_0 \rangle)}{dt} . \quad (2.6)$$

This is not an upper bound on the exact ground-state energy but is guaranteed to converge to it in the limit $t \to \infty$. As before, $E_{\phi\chi}(t)$ is expanded as a power series in t and Padé approximants are used as the series acceleration method.

B. Summary of previous applications

The t expansion has been applied to two-dimensional spin systems:[1] the Heisenberg antiferromagnet and the Ising model in $1+1$ dimensions. In the first case the connected coefficients were calculated up to t^7. The result obtained by Padé approximating the derivative is accurate to within an error range of 0.27% to 0.75% of the exact answer.

In the Ising model a mean-field variational state was used as the starting wave function $|\phi_0\rangle$. The expansion was carried out up to t^6, and the energy was calculated for a range of values of the variational parameter θ. Equation (2.2) turned out to be a function of two independent parameters, $E(t,\theta)$. For a fixed value of t the best upper bound on the exact ground-state energy was obtained minimizing $E(t,\theta)$ with respect to θ. Both the energy and the magnetization were very accurately reproduced, with a significant improvement over mean-field results.

The bistate contraction scheme was also applied to the Ising model[1] using the exact strong- and weak-coupling ground states as the starting wave functions $|\phi_0\rangle$ and $|\chi_0\rangle$. The energy, calculated to the same order in t as before, is less accurate than the variational treatment over the entire region in the coupling constant. This indicates the importance of a variational parameter in the method and below we will explore additional variational treatments.

The t expansion has also been applied to SU(2)- and SU(3)-lattice gauge theories in $3+1$ dimensions[2-6] computing the vacuum energy density, specific heat, string tension σ, mass of the lowest lying 0^{++}-glueball M and the ratio $R = M^2/\sigma$.

C. Present application

In the present work we apply the t expansion to the Lipkin model.[7,8] This is an exactly soluble two-level model suggested by Lipkin and co-workers[7] in order to test new approaches for the solution of the many-body problem. It involves two N-fold degenerate single-particle levels, separated by the single-particle energy ϵ, and N identical fermions. Two quantum numbers characterize a given single-particle state. One of them adopts the values $\sigma = -1$ (lower level) and $+1$ (upper level). The other, which may be called the p spin, singles out a state within the N-fold degeneracy.

We let p run from 1 to N and introduce the quasispin operators[7]

$$\begin{aligned} J_+ &= J_-^\dagger = \sum_p c_{p+}^\dagger c_{p-} , \\ J_z &= \tfrac{1}{2} \sum_{p\sigma} \sigma c_{p\sigma}^\dagger c_{p\sigma} , \end{aligned} \quad (2.7)$$

which fulfill the [SU(2)] angular momentum commutation rules.

The interaction is a monopole force scattering two particles from one level into the other. In terms of the quasispin operators (2.7) the Hamiltonian is written as

$$H = J_z + \frac{v}{2}(J_+^2 + J_-^2) , \quad (2.8)$$

where the energy is given in units of the single-particle energy ϵ. The ground state belongs, always, to the multiplet $J = N/2$ and therefore the exact solutions are found by diagonalizing a $2J+1 = N+1$ matrix.

The Hartree-Fock (HF) approach looks for the lowest state in the self-consistent representation which is obtained through a variation of the original basis. A phase transition is found[8] at $v_c = 1/(N-1)$. For $v < v_c$ the HF solution is the trivial one and the HF state coincides with the unperturbed ground state. In the full HF treatment the results for $E_{\rm HF}$ can be cast in terms of a single variational parameter β in the following way[8]

$$\begin{aligned} &\beta = 0, \quad E_{\rm HF} = -N/2 \quad \text{for } v \leq \frac{1}{N-1} , \\ &\cos\beta = \frac{1}{v(N-1)}, \quad E_{\rm HF} = -\frac{N}{2}\cos\beta - \frac{N}{4}\frac{\sin^2\beta}{\cos\beta} \\ &\qquad\qquad \text{for } v > \frac{1}{N-1} . \end{aligned} \quad (2.9)$$

For applying the t expansion one must calculate the connected matrix elements (2.4). This is straightforward when using one of the basis states $|J,M\rangle$ as the starting wave function $|\phi_0\rangle$. In particular we have used the unperturbed ground state $|N/2, -N/2\rangle$ which is a mean-field wave function because it corresponds to the HF state before the phase transition, i.e., in the weak-coupling regime.

Within nonrelativistic many-body theory there have been numerous suggestions for methods to produce a dynamical choice of the reference state $|\phi_0\rangle$.[9] We pro-

pose to use a simple dynamical vacuum generation method in conjunction with the t expansion. It consists in applying the Hamiltonian to the weak-coupling state used before, and keeping the two dominant components in the basis. We then label the two dominant components as $|1\rangle$ and $|2\rangle$, and we vary the one free amplitude in the new reference state

$$|\phi_0\rangle = \cos\theta\,|1\rangle + \sin\theta\,|2\rangle\ . \tag{2.10}$$

This method introduces a single variational parameter θ, which improves the results in a way analogous to Ref. 1.

Obviously, one could elect to keep the three, four, etc., largest components of the result obtained by acting with H on the reference state. Eventually, many variational parameters could be introduced so that the level of effort required approaches that of a HF treatment. However, the important distinction is that this dynamical basis method is not limited to a mean field approximation. It is to be noted that this approach is different from the bi-state contraction scheme suggested in Ref. 1 by virtue of preserving the energy $E(t,\theta)$ as an upper bound. This improvement arises due to the fact that there is a single (but multicomponent) starting wave function.

III. RESULTS

For obtaining the t expansion results in the Lipkin model we first take the unperturbed ground state as the reference state, $|\phi_0\rangle = |N/2, -N/2\rangle$, calculate the connected matrix elements (2.4) for the Hamiltonian (2.8) and so obtain the partial sums

$$S_L(t) = \sum_{m=0}^{L} \frac{\langle H^{m+1}\rangle^c}{m!}(-t)^m \tag{3.1}$$

that allow the construction of the Padé approximants[10] for any fixed value of t. It is to be noted that the calculation of the Padé $[M/M]$ requires the partial sum S_{2M}. Since one argues that the calculation has converged if several Padé approximants agree, we accept the maximum t value for which this occurs.

Different Padé results are shown in Figs. 1 and 2 for four and ten particles, respectively, and as functions of the coupling constant. The approximate energies are expressed as ratios with respect to the exact ground state energy and the HF results are also shown for comparison. It is clearly seen that the agreement with the exact results increases with the order of the Padé approximant considered, as it should. Even for low order Padé the results obtained are very good before and in the vicinity of the phase transition $[v(N-1)=1]$. In this region the t expansion results are better than the HF results. The t expansion results deviate more from the exact results with increasing values of v within the strong-coupling regime. This increasing deviation should be expected since we have chosen the unperturbed ground state as the reference state. This effect is even more important for larger N. Consequently, higher order Padé approximants are needed for larger values of v in order to get the same precision. One of the pecularities of the Lipkin model is that the HF energy tends to the exact ground state energy for $N\to\infty$ and $v\to\infty$. Thus, for sufficiently large N and v the HF result will be better than any fixed order Padé approximation to the t expansion based on the unperturbed HF solution as the reference state. Of course, the most logical procedure is to use the new HF state once one exceeds the critical coupling.

We have checked the consistency of our results by calculating the Padé approximants to the derivative given in (2.5) and verifying that the t value for which it goes to zero is the same as the one considered previously.

Next we consider the dynamical vacuum generation

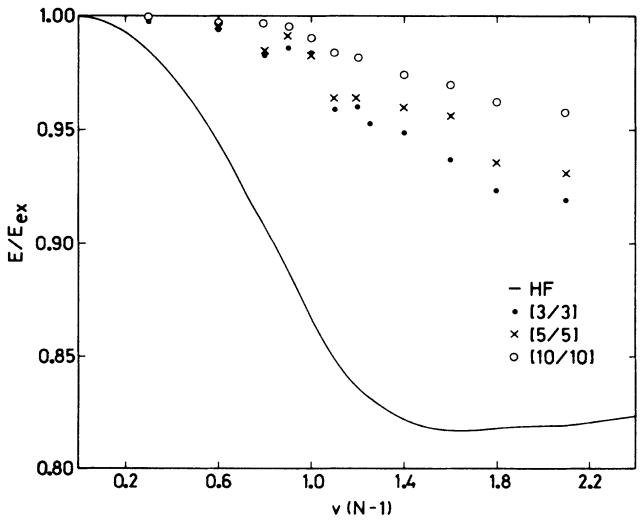

FIG. 1. Ratios of approximate energies with respect to the exact ground state energy as functions of the coupling constant for $N=4$. Discrete points signify the results obtained with $[M/M]$ Padé approximants to the series $E(t)$.

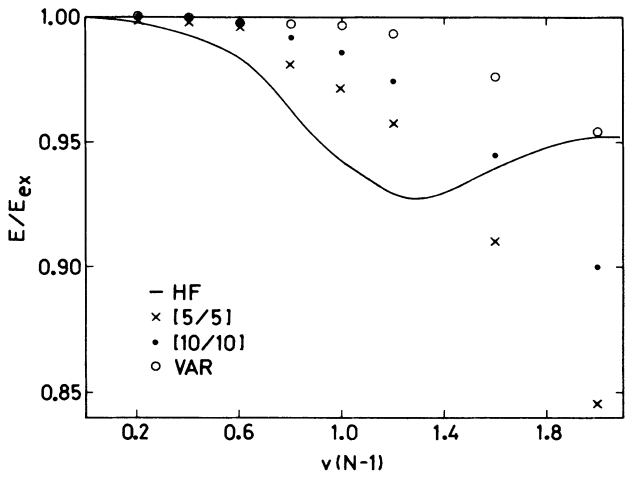

FIG. 2. Ratios of approximate energies with respect to the exact ground state energy as functions of the coupling constant for $N=10$. Discrete points, except circles, signify results obtained with $[M/M]$ Padé approximants to the series $E(t)$. Circles represent the results of varying θ after obtaining the [10/10] Padé approximant to $E(t,\theta)$.

method proposed in Sec. II C. Applying the Lipkin Hamiltonian (2.8) to the unperturbed ground state one goes to the same state and to a new one, $|N/2,-N/2+2\rangle$. Consequently, we take as the new reference state

$$|\phi_0\rangle=\cos\theta\left|\frac{N}{2},-\frac{N}{2}\right\rangle+\sin\theta\left|\frac{N}{2},-\frac{N}{2}+2\right\rangle \quad (3.2)$$

and recalculate the Padé approximants to the ground state energy as before but now as a function of θ. In the weak-coupling regime the minimum energy value is located at $\theta=0$ which, as expected, corresponds to the previous results. But when the coupling constant v increases the location of the minimum $E(t,\theta)$ for fixed t moves to larger values of θ. Typical values are around $\cos\theta=0.8$ for coupling constants of the order of twice the critical value as is shown in Fig. 3. The energy results obtained with this improved method are also shown in Fig. 2 for the [10/10] Padé.

The significant improvement obtained with a single variational parameter is remarkable. Notice that the behavior of this parameter is not expected to signal the phase transition as it is not a mean-field variational parameter. Motivated by the realization that it may be challenging to vary parameters of a dynamically determined vacuum in realistic situations, we investigated the hypothesis that it may be adequate to choose our single parameter θ by simply minimizing the first moment of the Hamiltonian, i.e., the energy expectation value $\langle\phi_0|H|\phi_0\rangle$. In the Lipkin model considered here this may be done analytically and yields the following result

$$\cos\theta=\left[\frac{1}{2}+\frac{1}{\sqrt{a+4}}\right]^{1/2},\qquad \sin\theta=-\left[\frac{1}{2}-\frac{1}{\sqrt{a+4}}\right]^{1/2}, \quad (3.3)$$

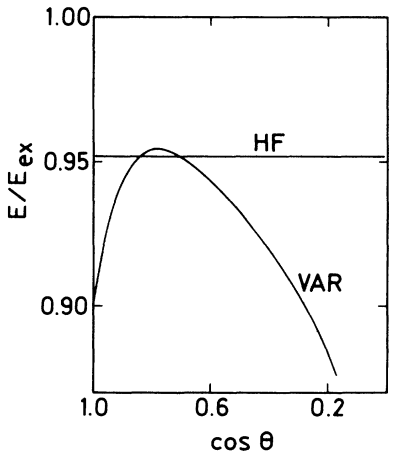

FIG. 3. Ratios of approximate energies with respect to the exact ground state energy as a function of the variational parameter for $N=10$ and $v(N-1)=1.98$. The curve named *VAR* corresponds to the results obtained with the [10/10] Padé approximant.

TABLE I. Exact and approximate results for the ground state and the first excited state energies, for $N=10$ and different values of the coupling constant.

$v(N-1)$	$\|5,-5\rangle$	E_{ex}(g.s.)	$\|5,-4\rangle$	E_{ex}(f.e.s.)
0.18	−5.008	−5.009	−4.020	−4.022
0.36	−5.032	−5.037	−4.079	−4.086
0.54	−5.072	−5.084	−4.176	−4.194
0.81	−5.154	−5.197	−4.365	−4.432
0.99	−5.229	−5.306	−4.540	−4.640
1.17	−5.303	−5.446	−4.716	−4.883
1.62	−5.624	−5.956	−5.214	−5.617
1.98	−5.873	−6.523	−5.625	−6.303

with $a=2N(N-1)v^2$.

After a Padé, the results are similar to the ones encountered by minimizing the Padé approximants themselves. A natural extension to obtain further improvements is to take a reference state with three or more components, having a corresponding number of variational parameters which are then fixed through the minimization of additional moments of the Hamiltonian.

Finally, we have examined the t-expansion method for the first excited state. We studied the results obtained when using as the reference state the unperturbed first excited state, $|\phi_0\rangle=|N/2,-N/2+1\rangle$. They are shown in Table I for $N=10$ and different values of the coupling constant. The Padé approximant used is [10/10]. We present the exact energies of the first excited state for comparison. To appreciate the quality of the t expansion results for the first excited state, we also show in Table I the results (obtained from $|\phi_0\rangle=|N/2,-N/2\rangle$) for the same Padé approximant to the exact ground state energies. It is remarkable that the t-expansion method provides ground state and first excited state results with the same precision requiring the same effort. Obviously this is due to the fact that in this simple model the first excited state has a different symmetry (parity) than the ground state and so we may easily choose a reference state that is always orthogonal to the ground state. By contrast, even in this simple case, the HF approach would require much more effort for providing an approximate first excited energy. Greater effort is required in HF, since one must either project states of different symmetry from the HF ground state or obtain the state of desired symmetry from the self-consistent solution of the HF equations with a constraint imposing orthogonality to the ground state.

IV. CONCLUSIONS

We may summarize the main conclusions of the present work as follows. The t expansion method works very well in the Lipkin model which is a standard testing ground for many-body theories of finite fermion systems. Starting with the weak-coupling mean-field wave function one gets very good results before and in the vicinity of the phase transition occurring in the model at the critical coupling constant $v_c=1/(N-1)$. One may also go beyond the phase transition, inside the strong-coupling region, without any problem. It is only when the number

of particles N and/or the coupling constant v are large that the t expansion results with the unperturbed HF state eventually deteriorate. Logically one should then switch to a new choice of the HF state in order to proceed even further into the strong coupling regime.

The dynamical vacuum generation method proposed in this work for constructing the starting wave function for the t expansion affects a major improvement in the approximate results in the strong coupling region without much additional effort. An interesting conclusion is that one may fix the variational parameter introduced in the vacuum by minimizing the first moment of the Hamiltonian before performing the t expansion. A natural and convenient extension for further improvements is to introduce more variational parameters to be fixed through the minimization of subsequent moments of the Hamiltonian. This extension of the t expansion method seems more promising, at least in the nuclear many-body problem, than the bistate contraction scheme proposed by Horn and Weinstein.[1]

We have shown that the t expansion method is capable of yielding first excited state energies with the same precision and comparable effort as the ground state energy. This success assumes an appropriate starting wave function with the correct symmetry is found. We have indicated how this is an advantage over some other variational approaches.

A final conclusion to be drawn from the results presented in this work is that a mean-field state is not required as the starting wave function to get good t expansion results. The only requirement is that the reference state $|\phi_0\rangle$ must have an overlap with the exact state one is trying to approximate. Calculating the overlaps between $|\phi_0\rangle$ and the exact solutions, which is simple in this soluble model, we have seen that the lower the overlap the greater the error in the approximate result for a fixed order Padé. Thus, the dynamical vacuum generation method proposed here is further motivated since it increases the overlap between the reference state and the exact solution. In particular, we have checked that the value of the parameter that provides the minimum energy, as shown in Fig. 3, corresponds to the point in which the overlap is maximum.

ACKNOWLEDGMENTS

We are pleased to acknowledge useful discussions with G. Bozzolo, D. Horn, M. Karliner, S. Klevansky, and M. Luban. It is also a pleasure to acknowledge the hospitality of the Santa Barbara Institute for Theoretical Physics where this work was initiated. M. C. C. is a fellow of the National Research Council of Argentina. She gratefully acknowledges support from the Organization of American States. This work was supported in part by the National Science Foundation Grant Nos. PHY82-17853, PHY85-05682, PHY86-04197, and INT84-13827, and by the U.S. Department of Energy under Contract No. DE-AC02-82ER40068, Grant No. DE-FG02-87ER40371 Division of High Energy and Nuclear Physics, and supplemented by funds from the National Aeronautics and Space Administration.

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