Analytic solution for the ground-state energy of the extensive many-body problem

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A closed form expression for the ground-state energy density of the general extensive many-body problem is given in terms of the Lanczos tridiagonal form of the Hamiltonian. Given the general expressions of the diagonal and off-diagonal elements of the Hamiltonian Lanczos matrix, $\alpha_n(N)$ and $\beta_n(N)$, asymptotic forms $\alpha(z)$ and $\beta(z)$ can be defined in terms of a parameter $z \equiv n/N$ (n is the Lanczos iteration and N is the size of the system). By application of theorems on the zeros of orthogonal polynomials we find the ground-state energy density in the bulk limit to be given, in general, by $\mathcal{E}_0 = \inf[\alpha(z) - 2\beta(z)]$. [S0163-1829(96)07044-0]

I. INTRODUCTION

Finding analytic means of calculating details of the energy spectrum of strongly interacting many-body systems has long been a goal of theoretical physics, with applications from low energy scales in condensed matter physics to high energy particle physics. In particular, accurate calculations of the ground-state energy are important to settle issues relating to the character of the ground state, or vacuum state, itself. While there has arisen a range of theoretical tools to tackle problems that cannot be treated by perturbation theory, many suffer from the effects of uncontrolled approximation to the extent that each, alone cannot be trusted to give a reliable answer. It is only when several independent methods point in the same direction, that one can confidently state something about the character of a system. Examples include mean-field theories neglecting correlations in fluctuations thereby reinforcing a tendency to order; exact diagonalization and Monte Carlo studies, at zero temperature, on relatively small clusters and the extrapolation to the bulk limit; finite temperature Monte Carlo simulation of somewhat larger systems, but at temperatures above the interesting low energy scales.

In this paper a simple fundamental relationship is found between the tridiagonal form of the Hamiltonian and the ground-state energy density. A general theorem is proved for the ground-state energy density in terms of the coefficients generated by the Lanczos method, evaluated in a limiting process incorporating convergence of the Lanczos iterates and the thermodynamic limit. The Lanczos method is based on the following recursion: starting from an appropriate trial state, one recursively generates new basis states with the repeated application of the Hamiltonian,

$$|v_n\rangle = \frac{1}{\beta_{n-1}}[(H-\alpha_{n-1})|v_{n-1}\rangle - \beta_{n-2}|v_{n-2}\rangle], \quad (1)$$

where $\alpha_n = \langle v_n|H|v_n\rangle$ and $\beta_n = \langle v_{n+1}|H|v_n\rangle$. At the nth iteration of this recursion the Hamiltonian matrix in the new basis of states is given by the tridiagonal, T_n, i.e.,

$$H \to T_n = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \ddots & \ddots & \\ & & \ddots & \alpha_{n-1} & \beta_{n-1} \\ & & & \beta_{n-1} & \alpha_n \end{bmatrix}. \quad (2)$$

The power of the Lanczos phenomenon is that the dimension of the tridiagonal basis, required to describe the low-lying states of the system, determined by the recursion level is significantly smaller than the original basis. The outermost eigenvalues of T_n rapidly converge to those of the Hamiltonian. In computing the Lanczos coefficients, α_n and β_n, exactly one is usually restricted to an early termination of the recursion in the analytic case treating large systems, or to small systems in a numerical calculation taken to complete convergence. To date all methods, however the Lanczos basis has been generated, require the numerical diagonalization of the tridiagonal T_n matrices for the ground-state energy. In this paper we will demonstrate how the diagonalization can be carried out analytically for extensive systems, thereby providing a solution for the ground-state energy density in terms of the tridiagonal form. By introducing a parameter, $z = n/N$, where N is the size of the system, the asymptotic forms $\alpha(z)$ and $\beta(z)$ are related to the ground-state energy by

$$\mathcal{E}_0 = \inf[\alpha(z) - 2\beta(z)]. \quad (3)$$

II. THERMODYNAMIC LIMIT OF THE TRIDIAGONAL FORM

Using the initial state, $|v_1\rangle$, one forms Hamiltonian moments, and from these the connected moments,

$$\langle H^n\rangle_c \equiv \langle v_1|H^n|v_1\rangle_c. \quad (4)$$

The connected moments encapsulate the essential physics of the system because they scale with the size of the system, N, as

$$\langle H^n\rangle_c \equiv c_n N. \tag{5}$$

Here N is a quantitative measure of the size of the system whether it be the number of sites in a lattice of localized spins, or the volume in a continuum model with itinerant particles. Although this form is restricted to the ground state or vacuum sector of the model, generalizations can be easily made to excited states.

A $1/N$ expansion of the Lanczos matrix elements, $\alpha_n(N)$ and $\beta_n(N)$, reveals a surprising analytic property—a simple polynomial n dependence. In terms of the connected coefficients c_n, this cluster expansion for the Hamiltonian *density* is[1,2]

$$\alpha_n(N) = c_1 + (n-1)\frac{1}{N}\left[\frac{c_3}{c_2}\right] + (n-1)(n-2)\frac{1}{N^2}\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{4c_2^4}\right] + O\left(\frac{1}{N^3}\right), \tag{6}$$

$$\beta_n^2(N) = \frac{n}{N}c_2 + n(n-1)\frac{1}{N^2}\left[\frac{c_2c_4 - c_3^2}{2c_2^2}\right] + n(n-1)(n-2)\frac{1}{N^3}\left[\frac{21c_2c_3^3c_4 - 12c_3^4 - 4c_2^2c_4^2 - 6c_2^2c_3c_5 + c_2^3c_6}{12c_2^5}\right] + O\left(\frac{1}{N^4}\right). \tag{7}$$

We first define a parameter $z \equiv n/N$ which remains finite as the Lanczos recursion proceeds in the bulk limit, $n\to\infty$ and $N\to\infty$. In this limit the expansions become a series in z, i.e.,

$$\alpha(z) \equiv \lim_{n,N\to\infty} \alpha_n(N) = c_1 + z\left[\frac{c_3}{c_2}\right] + z^2\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{4c_2^4}\right] + O(z^3), \tag{8}$$

$$\beta^2(z) \equiv \lim_{n,N\to\infty} \beta_n^2(N) = zc_2 + z^2\left[\frac{c_2c_4 - c_3^2}{2c_2^2}\right] + z^3\left[\frac{21c_2c_3^2c_4 - 12c_3^4 - 4c_2^2c_4^2 - 6c_2^2c_3c_5 + c_2^3c_6}{12c_2^5}\right] + O(z^4). \tag{9}$$

The cluster expansion guides us to the observation that, more generally, we have for the exact problem the asymptotic forms in the $n\to\infty$ and $N\to\infty$ regime,

$$\alpha_n(N) = \alpha(z) + O(1/N),$$

$$\beta_n^2(N) = \beta^2(z) + O(1/N). \tag{10}$$

We observe here a confluence of the two limiting regimes: that of convergence of the Lanczos iterates and of the thermodynamic limit into a single scaled Lanczos iteration number z.

III. ORTHOGONAL POLYNOMIALS AND VAN DOORN'S THEOREM

The connection between the Lanczos tridiagonal form of the Hamiltonian and the associated system of orthogonal polynomials is simple. The characteristic polynomial $D_n(x) = \det(T_n - xI_n)$ of the Lanczos tridiagonal matrix representation satisfies the following recursion relation:

$$D_n(x) = (\alpha_n - x)D_{n-1}(x) - \beta_{n-1}^2 D_{n-2}(x), \tag{11}$$

which in turn defines $P_n(x) \equiv (-1)^n D_n(x)$ as an orthogonal polynomial, the zeros of which are the eigenvalues of the T_n matrices. The analytic forms for the $\alpha_n(N)$ and $\beta_n(N)$ define a special class of orthogonal polynomials relevant to the many-body problem which are distinguished by a certain dependence on the size parameter N.

For the orthogonal polynomials $P_n(x)$ satisfying the recursion relation

$$P_n(x) = (x - \alpha_n)P_{n-1}(x) - \beta_{n-1}^2 P_{n-2}(x), \tag{12}$$

there exists a powerful theorem by Van Doorn[3] on the lower bound on the lowest zero which has been generalized by Ismail and Li[4] to include an upper bound to the largest zero. Simply stated, Ismail and Li's result is the following: if $x_k^{(1)}$ and $x_k^{(k)}$ are the smallest and largest zeros, respectively, of $P_k(x)$ with $k>1$ then they are bounded by the interval (A,B) where

$$A = \min\{f_n^- : 1 \leqslant n < k\},$$

$$B = \max\{f_n^+ : 1 \leqslant n < k\}, \tag{13}$$

and the bound sequence is given by

$$f_n^{\pm} = \frac{1}{2}\left[(\alpha_n + \alpha_{n+1}) \pm \left((\alpha_n - \alpha_{n+1})^2 + \frac{4}{a_n}\beta_n^2\right)^{1/2}\right]. \tag{14}$$

In the above expression for $f_n^{\pm}$, $\{a_n\}_1^{k-1}$ is a chain sequence. That is, there exists a parameter sequence $\{g_n\}_1^k$ for which we have the factorization of a_n,

$$a_n = g_{n+1}(1 - g_n), \quad 1 \leqslant n < k, \tag{15}$$

where $0 \leqslant g_1 < 1$ and $0 < g_n < 1$ for $1 < n \leqslant k$. Van Doorn's theorem is for strict equality, whereby maximizing the lower bound with respect to the parameter sequence gives the lowest eigenvalue exactly:

$$x_k^{(1)} = \max_{\{g\}}[\min_n\{f_n^- : 1 \leqslant n < k\}], \tag{16}$$

for $k>1$. Only a technical difference occurs with this theorem and the result of Ismail and Li in that $g_1=0$ and $g_k=1$.

For finite N the termination of the Lanczos recursion occurs at some $n_{\max}$ when the sector of Hilbert space, determined by the trial state, has been exhausted. In general, the basis of states grows faster than any linear enumeration with N. Taking the minimum of f_n^- to occur at some $\bar{n}=\bar{z}N$ ($\bar{n}<n_{\max}$), the asymptotic forms for $\alpha_n(N)$ and $\beta_n(N)$ give the leading order behavior of the lowest energy level as

$$x_{n_{\max}}^{(1)}=\max_{\{g\}}\left[\alpha(\bar{z})-\frac{1}{\sqrt{\alpha_{\bar{n}}}}\beta(\bar{z})+O(1/N)\right]. \tag{17}$$

Since $\beta_n(N)>0$, to maximize the right-hand side of the above expression with respect to the chain sequence we may choose the maximal constant chain sequence,[4]

$$a=\frac{1}{4\cos^2\left(\dfrac{\pi}{n_{\max}+2}\right)}. \tag{18}$$

We can now obtain the ground-state energy density $\mathcal{E}_0$, in the bulk limit:

$$\mathcal{E}_0=\lim_{N\to\infty}x_{n_{\max}}^{(1)}. \tag{19}$$

In the $N\to\infty$ limit, we also have $n_{\max}\to\infty$ giving $a\to 1/4$, and it is straightforward to establish that, in general, $\bar{z}$ is obtained by finding the greatest lower bound with respect to z. The ground-state energy density of the general extensive many-body problem in the bulk limit is therefore

$$\mathcal{E}_0=\inf_{z>0}[\alpha(z)-2\beta(z)]. \tag{20}$$

IV. EXAMPLES

As a first illustration of this exact analytic diagonalization of extensive systems, we consider the purely mathematical model defined by the tridiagonal form,

$$\alpha_n(N)=\left(1+\frac{an}{N^2}\right)^N,$$

$$\beta_n(N)=\left(1+\frac{bn}{N^2}\right)^N-1. \tag{21}$$

The lowest eigenvalue in the $N\to\infty$ limit is

$$\mathcal{E}_0=\inf[e^{az}-2e^{bz}+2]=\left(\frac{r}{2}\right)^{r/(1-r)}(1-r)+2,$$

where $r=a/b$. The minimum occurs at $z_{\min}=\ln(2/r)/b(r-1)$. It is a straightforward matter to numerically diagonalize this system for increasing N to demonstrate the convergence of the numerical results to the analytic expression. The results of this exercise are shown in Fig. 1 (for a typical case $a=3$ and $b=2$) where we plot the error, defined as the difference from the exact value, of numerical diagonalizations for increasing N. The approach to the analytic solution is clear as $N\to\infty$.

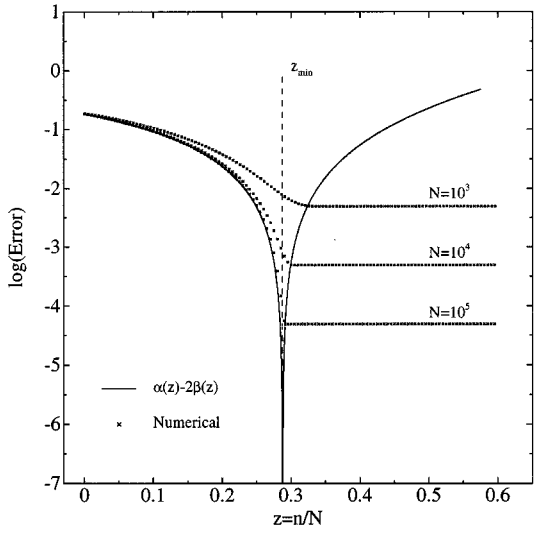

FIG. 1. Comparison of the analytic solution with numerical diagonalization for the simple case, $\alpha_n(N)=(1+an/N^2)^N$ and $\beta_n(N)=(1+bn/N^2)^N-1$, with $a=3$ and $b=2$.

Second, we compare the analytic diagonalization with numerical results using the truncated Lanczos coefficients given by the plaquette expansion. We do this here for the case of the antiferromagnetic Heisenberg chain, for which the expansions have been derived to high order using the classical Néel state as the trial state. This state is a poor choice for the isotropic Heisenberg model but is sufficiently simple to allow the computation of moments up to $\langle H^{28}\rangle_c$. Employing the traditional analysis of the plaquette expansion the T_n matrices are diagonalized numerically for increasing chain size N.[5] In Figs. 2 and 3 we demonstrate the approach of the numerical diagonalization for the ground state to the analytic expression as the $N\to\infty$ limit is approached. We show the two typical cases which can occur due to the trun-

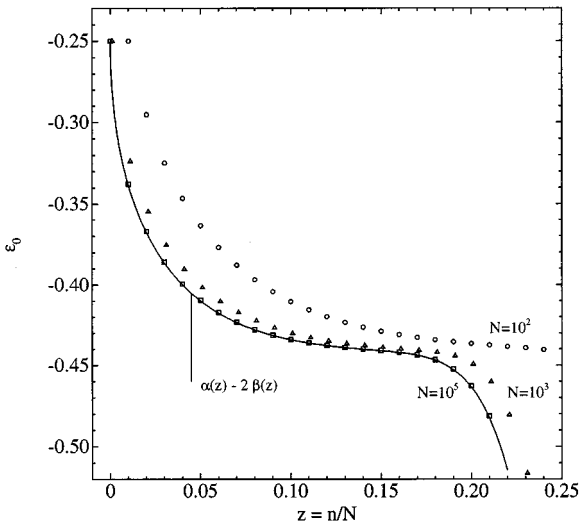

FIG. 2. Plaquette expansion of the one-dimensional (1D) antiferromagnetic Heisenberg model at an order $(1/N^{11})$ where a point of inflection develops due to the breakdown of the expansion. The numerical diagonalization for increasing N converges to the function $\alpha(z)-2\beta(z)$.

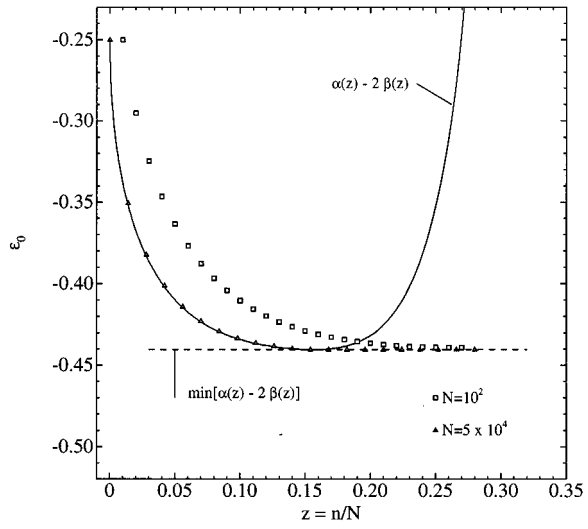

FIG. 3. Plaquette expansion of the 1D antiferromagnetic Heisenberg model at an order $(1/N^7)$ where a minimum develops in $\alpha(z)-2\beta(z)$. The numerical diagonalization data at $N=5\times10^4$ clearly display the convergence to the value of $\min[\alpha(z)-2\beta(z)]$.

cation of the expansions for $\alpha(z)$ and $\beta(z)$. Figure 2 corresponds to an order of the plaquette expansion for which $\alpha(z)-2\beta(z)$ has no minimum—a point of inflection develops, reflecting the fact that the expansion naturally breaks down at some large enough value of z. Figure 3 shows a case where a minimum develops—the numerical values for the lowest eigenvalue in the large volume limit match onto the value at the minimum.

We must emphasize that the plaquette expansion is a series expansion of the exact Lanczos coefficients about $z=0$ and truncated, and is therefore only reliable for small z. The error involved grows rapidly with z which can occur with either sign, and thus the large z behavior of the truncated approximations bear no relation to the exact behavior. Because of this we do not expect that at every order at which the truncation is made that a minima would arise.

V. CONCLUSIONS

We have found an expression for the ground-state energy density for the extensive many-body problem which is completely general and, since the Hamiltonian was diagonalized exactly, is nonperturbative. Given the Hamiltonian in tridiagonal form the expression can be used immediately. So far, the exact analytic transformation of a system to tridiagonal form has not been achieved for any examples of solvable systems. This state of affairs may change as the theorem proved here gives impetus to efforts in this direction. However, an immediate approximate tridiagonalization of the general problem does exist in the plaquette expansion and studies of the usefulness of this method with better trial states also merit further work. The analytic nature of this expansion uncovered the existence of the scaled Lanczos iteration parameter $z=n/N$ and the asymptotic forms $\alpha(z)$ and $\beta(z)$ for the exact problem.

An interesting extension of this work is to consider a similar analysis on excited states. An indication that the solution for the mass gap of the general extensive many-body system may, in fact, be possible is the fact that the mass gap of the first order plaquette expansion has already been solved analytically.[6,7] Such a generalization is presently under active investigation.

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