General nonperturbative estimate of the energy density of lattice Hamiltonians

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Employing a theorem on lower bounds on the zeros of orthogonal polynomials, the plaquette expansion to order $1/N_p$ of the tridiagonal Lanczos matrix elements is solved for the ground-state energy density in the infinite lattice limit. The resulting nonperturbative expression for the estimate of the energy density in terms of the connected coefficients to order $\langle H^4\rangle_c$ is completely general. This expression is applied to various Hamiltonian systems—the Heisenberg model in D dimensions and SU(2) and SU(3) lattice gauge theory in $3+1$ dimensions. In all cases the analytic estimate to the energy density is not only a significant improvement on the trial state, but is typically accurate to a few percent. The energy density of the D-dimensional Heisenberg model is predicted to approach $\mathcal{E}_0(\text{Néel})-\frac{1}{8}$ for large D. In the case of SU(2) and SU(3) the specific heat derived from the energy density peaks at the correct strong- to weak-coupling transition.

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I. INTRODUCTION

A straightforward technique to find the eigenstates of many-body systems is to transform the Hamiltonian iteratively using the Lanczos method into tridiagonal form, from which the eigenstates can be computed numerically. The tridiagonal basis is constructed with respect to some well-chosen starting state $|v_1\rangle$ in the appropriate sector of the Hilbert space, according to the Lanczos recursion:

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

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 takes the form

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

Diagonalization of the tridiagonal matrices T_n gives eigenstates which rapidly converge to the low-lying states of the original Hamiltonian (up to an orthogonal transformation).

In the calculation of the Lanczos coefficients α_n and β_n one is limited to either a numeric computation of a large number of iterations for small bases or an analytic calculation for only the first few iterations. The many-body limit can only be reached by extrapolation. However, it is now known [1,2] that these matrix elements for a Hamiltonian defined on a lattice of N_p plaquettes admits a cluster expansion:

$$\begin{aligned}\alpha_n&=N_pc_1+(n-1)\left[\frac{c_3}{c_2}\right]+\tfrac{1}{2}(n-1)(n-2)\left[\frac{3c_3^3-4c_2c_3c_4+c_2^2c_5}{2c_2^4}\right]\frac{1}{N_p}+\cdots\,,\\ \beta_n^2&=nc_2N_p+\tfrac{1}{2}n(n-1)\left[\frac{c_2c_4-c_3^2}{c_2^2}\right]+\tfrac{1}{6}n(n-1)(n-2)\left[\frac{-12c_3^4+21c_2c_3^2c_4-4c_2^2c_4^2-6c_2^2c_3c_5+c_2^3c_6}{2c_2^5}\right]\frac{1}{N_p}+\cdots\,,\end{aligned} \tag{3}$$

where the c_n are given by the connected [3] Hamiltonian moments $\langle H^n\rangle_c\equiv c_nN_p$ with respect to the trial state $|v_1\rangle$. The above plaquette expansions for α_n and β_n have been used to numerically calculate the energy density of various models [1,4] in the infinite lattice limit for increasing orders in $1/N_p$. In contrast with most methods in many-body systems these calculations work directly in the large lattice limit—in the process of Lanczos iteration a fraction of order 1 of the N_p sites is coupled by the modified interaction determined by the maximum order of connected Hamiltonian moments. The Hamiltonian matrix is diagonalized numerically and the infinite lattice limit taken. The only approximation is the initial truncation of the plaquette expansion.

There are many remarkable properties of this symmetric tridiagonal form yet to be investigated analytical-

ly. One of the most important properties is that the characteristic polynomial of the matrix T_n is an orthogonal polynomial—the particular form of the plaquette expansion to a given order defines a system of orthogonal polynomials. Hence the plaquette expansion reduces the problem of calculating the spectrum by diagonalization to that of calculating (possibly analytically) the zeros of a system of orthogonal polynomials. It is important to realize that the plaquette expansion is completely general and the system of orthogonal polynomials relevant to this problem is the same for all Hamiltonians.

In this paper we consider the plaquette expansion of the Hamiltonian density to order $1/N_p$ and demonstrate that using theorems on the properties of the extreme zeros of orthogonal polynomials an analytic solution for the energy density in the $N_p \to \infty$ limit can be found for this order. To demonstrate the power of this analytic estimate we use this solution to compute the ground-state energy density of the D-dimensional Heisenberg model and of SU(2) and SU(3) lattice gauge theories in $3+1$ dimensions.

II. FIRST-ORDER SYSTEM

Before we consider the specific case of the $O(1/N_p)$ expansion we will outline the connection between the Lanczos tridiagonal form of the Hamiltonian and the associated system of orthogonal polynomials. The characteristic polynomial $D_n(x)=\det(T_n - xI_n)$ of the Lanczos tridiagonal matrix satisfies the recursion relation

$$D_n(x)=(\alpha_n - x)D_{n-1}(x)-\beta_{n-1}^2 D_{n-2}(x) , \tag{4}$$

which in turn defines $(-1)^n D_n(x)$ as an orthogonal polynomial. There are many useful properties of orthogonal polynomials and powerful theorems on the zeros. For the orthogonal polynomial $P_n(x)\equiv(-1)^n D_n(x)$ satisfying the recursion relation

$$P_n(x)=(x-\alpha_n)P_{n-1}(x)-\beta_{n-1}^2 P_{n-2}(x) , \tag{5}$$

we use a theorem by van Doorn [5] on the lower bound on the lowest zero which has been generalized by Ismail and Li [6] to include an upper bound to the largest zero.

If $x_N^{(1)}$ and $x_N^{(N)}$ are the smallest and largest zeros, respectively, of $P_N(x)$ then they are bounded by the interval (A,B) where

$$\begin{aligned} A &= \min\{x_n^- : 1<n<N\} , \\ B &= \max\{x_n^+ : 1<n<N\} , \end{aligned} \tag{6}$$

and the bound sequence is given by

$$x_n^{\pm}=\tfrac{1}{2}\left[(\alpha_n+\alpha_{n+1})\pm\left[(\alpha_n-\alpha_{n+1})^2+\frac{4}{a_n}\beta_n^2\right]^{1/2}\right] . \tag{7}$$

In the above expression for $x_n^{\pm}$, $\{a_n\}_1^N$ is a chain sequence. That is, there exists a parameter sequence $\{g_n\}_0^N$ for which we have the factorization of a_n:

$$\begin{aligned} &a_n=g_n(1-g_{n-1}),\quad 0<n\le N,\quad 0\le g_0<1 , \\ &0<g_n<1,\quad 0<n\le N . \end{aligned} \tag{8}$$

The lower bound is improved by choosing a maximal chain sequence.

This bound can be applied immediately to the plaquette expansion with startling results. First, in order to simplify the notation, the $O(1/N_p)$ plaquette expansion is rewritten as

$$\begin{aligned} \alpha_n &= \frac{b}{\sqrt{c}}\frac{n-1}{N_p} , \\ \beta_n^2 &= \sqrt{c}\,\frac{n}{N_p}+a\frac{n(n-1)}{N_p^2} , \end{aligned} \tag{9}$$

where we are now working with the Hamiltonian density H/N_p and have set c_1 to zero without loss of generality (since c_1 only defines the zero of energy). The reason for the above choice of parametrization will become apparent. The minimum value of the bound function can be found quite simply and the limit $N_p \to \infty$ taken. One finds

$$\lim_{N_p\to\infty} A=\frac{1}{2a}\left[\left[b^2-\frac{ac}{a_n}\right]^{1/2}-b\right] . \tag{10}$$

This value of A represents a set of lower bounds, depending on the value of the chain parameter a_n, on the zeros of the characteristic polynomials in the $N_p \to \infty$ limit.

We find that using the maximum value of a constant chain sequence [6], $a_n=\frac{1}{4}$, the upper and lower bounds correspond *exactly* to the actual largest and smallest zeros of the $O(1/N_p)$ system. In other words the solution of the ground-state energy density $\mathcal{E}_0$ from the $O(1/N_p)$ plaquette expansion is

$$\mathcal{E}_0=\frac{1}{2a}[-b+\sqrt{b^2-4ac}\,] . \tag{11}$$

This expression is valid for all $a<0$ and for $a>0$ when $b^2-4ac>0$. For the case where $a<0$ the spectrum is bounded above by

$$\mathcal{E}_{\max}=\frac{1}{2a}[-b-\sqrt{b^2-4ac}\,] . \tag{12}$$

However, for the case $a>0$ (with $b^2-4ac>0$), rather than the ground-state solution changing to the other root, the expression for $\mathcal{E}_{\max}$ is no longer valid, however, the ground-state energy density is still given by Eq. (12).

In terms of the connected coefficients the solution to the $O(1/N_p)$ plaquette expansion gives an estimate to the energy density of the original Hamiltonian,

$$\mathcal{E}_0=c_1+\frac{c_2^2}{c_2c_4-c_3^2}[\sqrt{3c_3^2-2c_2c_4}-c_3] , \tag{13}$$

with the condition

$$\Delta\equiv 3c_3^2-2c_2c_4>0 . \tag{14}$$

That the lower bound, Eq. (12), is the actual ground state of the $O(1/N_p)$ system can be proved by considering an alternative upper bound to the lowest zero:

$$x_n^{(1)}\le\sqrt{||T_n v_k||^2} , \tag{15}$$

where v_k is a normalized vector with zero in the first $n-k$ positions and unity in the remainder [6]. This upper bound on the lowest zero coincides with the lower bound equation (12) when the limits $n \to \infty$ and $k \to \infty$ are suitably taken together with $N_p \to \infty$.

It may be possible to carry out this bound analysis for higher orders in the plaquette expansion and obtain systematically more accurate expressions for the ground-state energy density. In the interim we will show with a few examples that the solution of the $O(1/N_p)$ plaquette expansion is typically accurate to a few percent.

III. ANTIFERROMAGNETIC HEISENBERG MODEL IN D DIMENSIONS

The Heisenberg model a lattice of N spins is defined by the Hamiltonian

$$H = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \ , \tag{16}$$

where the summation is over nearest neighbors and periodic boundary conditions are adopted ($N_p = N$). We have calculated the connected coefficients for the D-dimensional hypercubic lattice with respect to the Néel state to be

$$\begin{aligned} c_1(D) &= -\frac{D}{4} \ , \\ c_2(D) &= \frac{D}{4} \ , \\ c_3(D) &= \frac{D}{4}(2D-1) \ , \\ c_4(D) &= \frac{D}{8}(8D^2-10D+1) \ , \end{aligned} \tag{17}$$

with $\Delta(D) > 0$ for all D.

The first-order plaquette expansion estimate to the energy density from Eq. (14) is

$$\mathcal{E}_0(D) = \frac{2D^2-3D-2D\sqrt{4D^2-2D+2}}{8D+4} \ , \tag{18}$$

which has the interesting limit $\mathcal{E}_0(D) = \mathcal{E}_0(\text{Néel}) - \frac{1}{8}$ as $D \to \infty$ as shown in Fig. 1. Values of the estimate for small D are given in Table I. The exact results for $D=1$ and $D=2$ indicate the accuracy of the estimate. For $D=3$ the energy density is not as accurately known and so we give a range of values from the literature [12] for comparison.

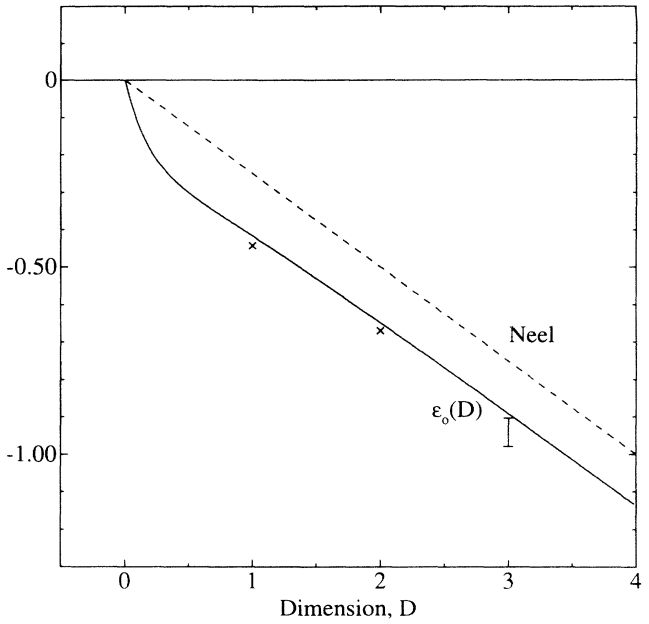

FIG. 1. Analytic estimate $\mathcal{E}_0(D)$ for the D-dimensional antiferromagnetic Heisenberg model. Also shown is the Néel energy density for each dimension. The crosses are the exact results for $D=1$ and $D=2$. For $D=3$ the exact result is not well known and so we give a range of values found in the literature [12].

IV. SU(2) LATTICE GAUGE THEORY

The Kogut-Susskind SU(2) lattice Hamiltonian in 3+1 dimensions is given by [7]

$$H = \frac{g^2}{2} \sum_l \mathbf{E}_l^2 + \frac{2}{g^2} \sum_p (2 - \mathrm{tr} U_p) \ , \tag{19}$$

where $\mathbf{E}_l$ is the color electric flux operator corresponding to the link l, $\mathrm{tr}U_p$ is the magnetic flux operator corresponding to the plaquette p, and g is the coupling constant. The connected moments have been calculated in the vacuum sector by Mathews, Snyderman, and Bloom [8] with respect to the strong-coupling state:

$$\begin{aligned} c_1 &= 2y \ , \\ c_2 &= y^2 \ , \\ c_3 &= 3y \ , \\ c_4 &= 9 - y^4 \ , \end{aligned} \tag{20}$$

TABLE I. Analytic approximation $\mathcal{E}_0(D)$ for the D-dimensional Heisenberg model and comparison with numeric results for low dimensions.

D	$\mathcal{E}_0(D)$	Comparison	
1	$-\frac{5}{12} = -0.4166$	-0.44315	Exact
2	$(1-2\sqrt{14})/10 = -0.6483$	$-0.66934(3)$	(Monte Carlo [11])
3	$3(3-8\sqrt{2})/28 = -0.8908$	$-0.9028 \to -0.9785$	(Various [12])

with $y=2/g^2$ and $\Delta(y)>0$ for all y.

The energy density estimate for the vacuum takes the form

$$\mathcal{E}_0(y)=\frac{1}{y}[2y^2+3-\sqrt{9+2y^4}]\ . \tag{21}$$

In Fig. 2 we plot this approximation to the energy density of pure SU(2) gauge theory together with the "specific heat" $C_v\equiv-\partial^2\mathcal{E}_0/\partial y^2$. As expected, the energy density derived from the strong-coupling state matches the strong-coupling limit precisely, but becomes less accurate at weak coupling where the specific heat becomes negative. However, even this first-order estimate is accurate enough to predict the strong to weak transition as is evident from the peaking behavior of C_v at $y=1$ which agrees with the t-expansion analysis [9].

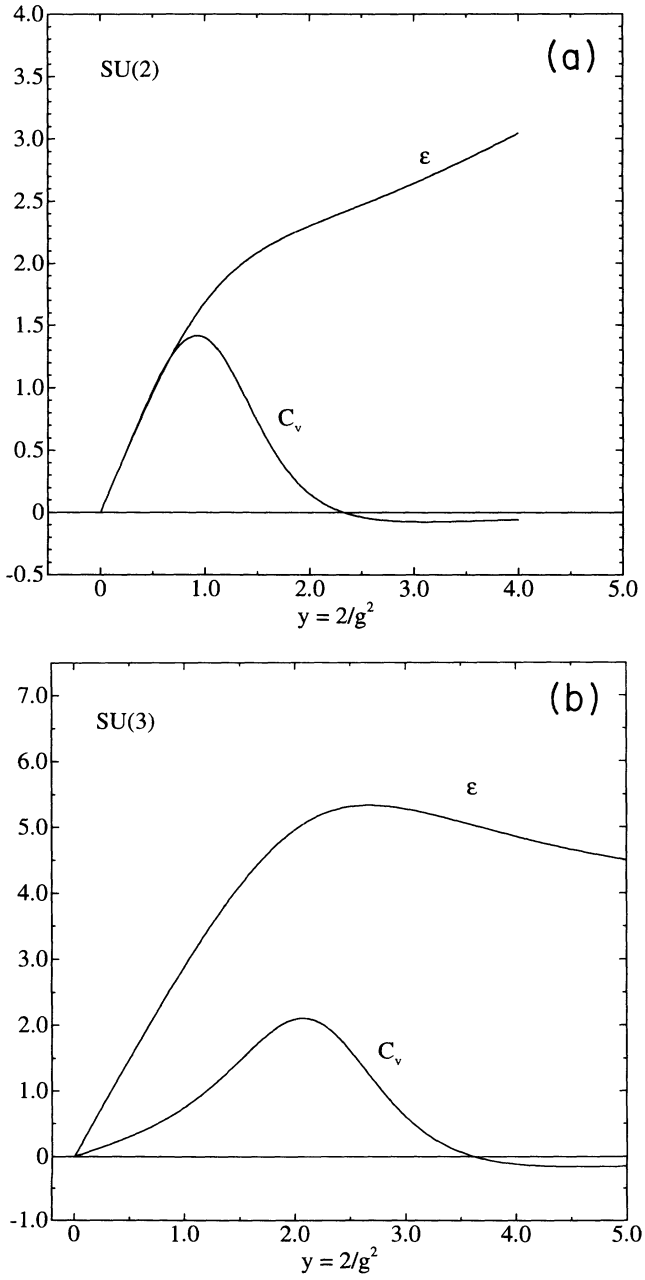

FIG. 2. Analytic estimate $\mathcal{E}_0(y)$ for (a) SU(2) and (b) SU(3) lattice gauge theories. The specific heat $C_v=-\partial^2\mathcal{E}_0/\partial y^2$ is also plotted for both theories.

V. SU(3) LATTICE GAUGE THEORY

In analogous notation to the SU(2) case, the Kogut-Susskind SU(3) lattice Hamiltonian in $3+1$ dimensions is

$$H=\frac{g^2}{2}\sum_l \mathbf{E}_l^2+\frac{1}{g^2}\sum_p(6-\mathrm{tr}U_p-\mathrm{tr}U_p^\dagger)\ . \tag{22}$$

From the strong-coupling state in the vacuum sector the connected Hamiltonian moments are [10]

$$\begin{aligned} c_1&=3y\ ,\\ c_2&=\frac{y^2}{2}\ ,\\ c_3&=-\frac{y^3}{4}+\frac{8y}{3}\ ,\\ c_4&=-\frac{8y^2}{3}+\frac{128}{9}\ , \end{aligned} \tag{23}$$

where again we have $y=2/g^2$ and $\Delta(y)>0$ for all y.

For SU(3) the energy density estimate becomes

$$\mathcal{E}_0(y)=\frac{1}{3y}[6y^2+32-\sqrt{1024-192y^2+27y^4}]\ . \tag{24}$$

We plot the energy density and the specific heat for SU(3) in Fig. 2. The quality of the results is similar to the SU(2) case with the specific-heat peaking in the strong- to weak-coupling transition region, again in agreement with the t-expansion analysis [10].

VI. CONCLUSION

In this work we have solved the first-order plaquette expansion of many-body systems in general. The resulting analytic estimate of the energy density on the bulk limit is quite powerful as it relies on only calculating the Hamiltonian moments up to fourth order and yet appears to be accurate in the nontrivial systems considered here.

The energy density estimate presented here is not just of use in the vacuum sector. By using a trial state in a different sector of Hilbert space one obtains the lowest energy state in that sector. Subtraction of the vacuum energy gives an estimate to the mass gap of that sector.

Furthermore, this energy estimate can be used as a basis for a higher order variational technique when used in conjunction with a variational trial state.

The success of the first-order plaquette expansion solution leads one to ask whether the next order can be solved analytically. Given the simple form of the bound function this may indeed be the case. Work in this direction is in progress.

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