Plaquette expansion of the two-dimensional antiferromagnetic Heisenberg model

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The plaquette expansion of the Lanczos recursion method is applied to the two-dimensional antiferromagnetic Heisenberg model. Connected Hamiltonian moments $\langle H^n\rangle_c$ are calculated with respect to the Néel state up to $n=6$. The subsequent plaquette expansion of the Lanczos matrix in the number of plaquettes on the lattice, N_p, is determined to order $1/N_p$. Diagonalizing the Lanczos matrix in this form gives a value of the energy density of -0.664 in the limit $N_p\to\infty$, in good agreement with existing calculations.

I. INTRODUCTION

It has recently been observed[1] that for lattice models the Lanczos recursion applied in operator form admits a cluster expansion of the Lanczos matrix elements α_n and β_n. This expansion in the number of plaquettes on the lattice, N_p, gives the Hamiltonian in tridiagonal form analytically up to working order in the expansion and provides a method of calculating the spectrum of lattice models in the infinite lattice limit. An outline of the plaquette expansion is as follows.

From the Lanczos recursion relation with respect to some initial trial state $|v_1\rangle$,

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

one can derive expressions for the first few α_n and β_n in terms of Hamiltonian moments, $\langle H^n\rangle\equiv\langle v_1|H^n|v_1\rangle$, in a straightforward manner. By the time one gets as far as the sixth iteration (i.e., up to α_6 and β_5), the algebra has become too complex to continue. Plaquette dependence is introduced by writing the $\langle H^n\rangle$ in terms of connected Hamiltonian moments which scale with the number of plaquettes as $\langle H^n\rangle_c=c_nN_p$. The expressions for $\alpha_{1\to6}$ and $\beta_{1\to5}$ can be expanded in $1/N_p$. A clear structure becomes apparent from which one can infer a general plaquette expansion for the Lanczos matrix elements,

$$\begin{aligned}\alpha_n&=N_p\left[a_0+(n-1)\frac{a_1}{N_p}+(n-1)(n-2)\frac{a_2}{N_p^2}+\cdots\right]\ ,\\ \beta_n^2&=N_p\left[nb_0+n(n-1)\frac{b_1}{N_p}\right.\\ &\qquad\left.+n(n-1)(n-2)\frac{b_2}{N_p^2}+\cdots\right]\ ,\end{aligned} \tag{2}$$

where the coefficient functions are given by

$$\begin{aligned}a_0&=c_1\ ,\\ a_1&=\frac{c_3}{c_2}\ ,\\ a_2&=\frac{3c_3^3-4c_2c_3c_4+c_2^2c_5}{4c_2^4}\ ,\\ b_0&=c_2\ ,\\ b_1&=\frac{c_2c_4-c_3^2}{2c_2^2}\ ,\\ b_2&=\frac{-12c_3^4+21c_2c_3^2c_4-4c_2^2c_4^2-6c_2^2c_3c_5+c_2^3c_6}{12c_2^5}\ .\end{aligned} \tag{3}$$

The plaquette expansion is a combinatoric feature of the Lanczos recursion itself—no assumptions were made concerning the physics on lattice, only the existence of the connected moments. Working with specific models, higher-order terms in the expansion can be inferred. Furthermore, if one constructs the set of Lanczos matrices corresponding to plaquette expansions of α_n and β_n to order $1/N_p^r$ and computes the lowest eigenvalue (at a value of n before the expansion breaks down), $\lambda_0^{(r)}(N_p)$, one finds that the energy density is finite in the infinite lattice limit: i.e.,

$$\lim_{N_p\to\infty}\frac{\lambda_0^{(r)}(N_p)}{N_p}=\mathcal{E}_0^{(r)}\ . \tag{4}$$

In the cases studied so far, the energy densities $\mathcal{E}_0^{(r)}$ form a sequence of approximates which clearly approach the ground-state energy density in the infinite lattice limit. For the one-dimensional Heisenberg model, $\mathcal{E}_0^{(5)}$ is within about 0.1% of the true answer,[2] while for the XY model[2] the convergence was not as fast and $\mathcal{E}_0^{(5)}$ was found to be within 1% of the true answer (indicating an inefficient choice of trial state in those calculations).

In this work we apply the plaquette expansion to the case of the two-dimensional (2D) antiferromagnetic Heisenberg (AH) model. The importance of this model in the physics of CuO planes of the high-T_c superconductors has led to a number of detailed calculations of the

ground-state energy density, and hence we are well poised to compute this quantity using the plaquette expansion and compare with existing calculations.

II. APPLICATION TO THE 2D HEISENBERG MODEL

The Heisenberg model in two dimensions on a lattice of N spins is defined by the Hamiltonian

$$H=\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\ , \tag{5}$$

where the summation is over nearest neighbors. We adopt periodic boundary conditions ($N_p=N$).

To obtain the plaquette expansion, it is necessary to calculate the connected Hamiltonian moments with respect to a trial state $|v_1\rangle$ suitable for the state of interest. For our purposes the trial state must have some overlap with the true ground state of the system; hence, we choose the Néel state for simplicity. Calculation of the connected moments is facilitated in the following way. On a lattice of size $L\times L$ (L even, $N=L^2$ spins), the states

$$|\psi_p\rangle=H^p|\phi_0\rangle \tag{6}$$

are constructed for $p\le L/2-1$. The products give the Hamiltonian moments

$$\langle\psi_p|\psi_q\rangle=\langle H^{p+q}\rangle \tag{7}$$

up to order $p+q\le L-2$ for a lattice with $N_p=L^2$ plaquettes. One then extracts the connected moments $\langle H^n\rangle_c=c_nN_p$, where the connected coefficients c_n ($n\le L-2$) are independent of the lattice size (calculation of c_L in this way would suffer from boundary effects). The maximum lattice size used was 8×8 for which connected coefficients up to $n=6$ were calculated. These value are given in Table I.

III. RESULTS AND DISCUSSION

Using these values for c_n, we obtain the plaquette expansion for α_n and β_n up to $1/N_p$. Labeling the ground-state eigenvalue of the lth Lanczos iteration corresponding to the expansion to $1/N_p^r$ ($r=0,1$) as $\lambda_0^{(r)}(l,N_p)$, we examine this quantity as a function of l. In Fig. 1 a typical case is depicted showing a clear convergence region (for both $r=0$ and 1). For each expansion order r, we define an upper bound to the ground-state energy $E_0^{(r)}(N_p)$ to be the value of $\lambda_0^{(r)}(l,N_p)$ at the point of inflection l_i (or where convergence has occurred). Figure 2 shows the N_p dependence of the ground-state energy density upper bounds, $E_0^{(r)}(N_p)/N_p$. In particular, the

TABLE I. Connected coefficients for the AH model in 2D with respect to the Néel state.

n	1	2	3	4	5	6
c_n	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{13}{4}$	-7	$-\frac{635}{4}$

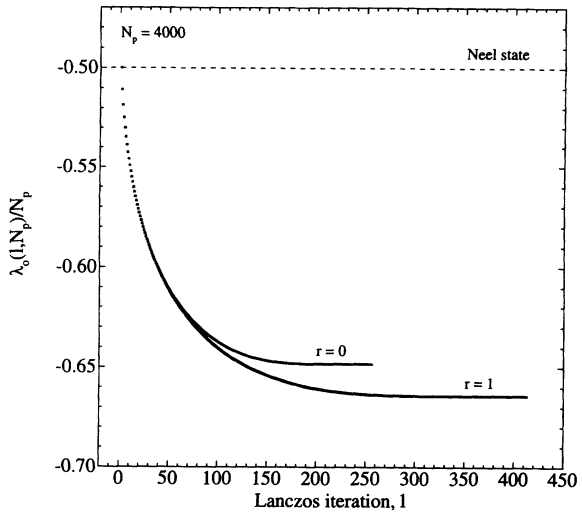

FIG. 1. Ground-state energy density $\lambda_0^{(r)}(l,N)/N$ (r is the truncation order) as a function of Lanczos iteration l. The data shown are for $N_p=4000$.

$N_p\to\infty$ behavior clearly shows the existence of a finite limit $\mathcal{E}_0^{(r)}$ for the ground-state energy density corresponding to each order r. At $N_p=4000$ where convergence has occurred we find

$$\begin{aligned}\mathcal{E}_0^{(0)}&=-0.648\ ,\\ \mathcal{E}_0^{(1)}&=-0.664\ .\end{aligned} \tag{8}$$

The model has been studied by many authors[3] using methods such as Monte Carlo,[4] Lanczos diagonalization of finite lattices,[5] variational techniques,[6] spin-wave theory[7] and series expansion.[8] While there have been many calculations of the ground-state energy density over the years—the values in the literature vary between

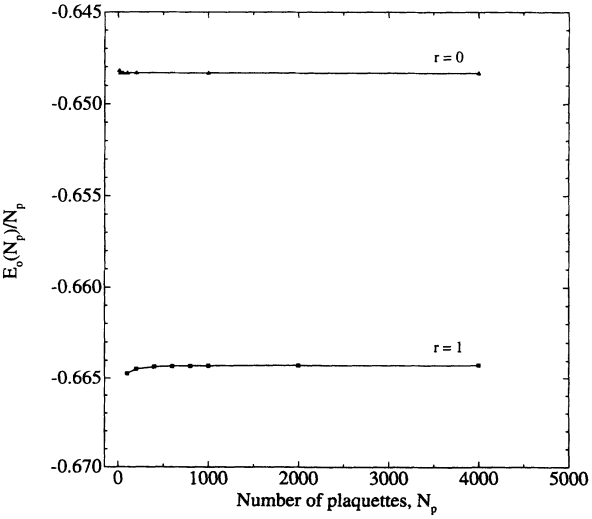

FIG. 2. Behavior of the ground-state energy density $E_0^{(r)}(N_p)/N_p$ in the large lattice limit $N_p\to\infty$.

-0.64 and -0.67—there has recently been agreement to high precision, in particular, a series calculation by Weihong, Oitmaa, and Hamer[8] giving $\mathcal{E}_0=-0.6693(1)$ and a Green's function Monte Carlo calculation by Runge[4] giving $\mathcal{E}_0=-0.669\,34(3)$.

It appears that the plaquette expansion result to $O(1/N_p)$ is already to the exact value. It should be emphasized that, given the c_n, the amount of computational effort required is negligible (i.e., the diagonalization of a 4000×4000 tridiagonal matrix in this case). Furthermore, the plaquette expansion calculates directly in the bulk limit and requires no extrapolation to $N_p\rightarrow\infty$. The agreement of the plaquette expansion result with the exact value not only lends credibility to the method, but also indicates that the Néel state must have significant overlap with the true ground state.

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