Plaquette expansion in lattice Hamiltonian models

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The Lanczos method in operator form is applied to a general lattice Hamiltonian and expressions for the first few Lanczos matrices in terms of the connected Hamiltonian moments $\langle H^n \rangle_c$ and the number of plaquettes, N_p, are obtained. Expansions in $1/N_p$ suggest a very simple general form for the first few terms in the $1/N_p$ expansions for all α_n and β_n. For the one-dimensional Heisenberg spin chain it is demonstrated that the ground-state eigenvalue of the tridiagonal Lanczos matrix derived from this plaquette expansion approaches the true infinite lattice limit as the number of terms in the plaquette expansion is increased.

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The calculation of the spectrum of quantum chromodynamics (QCD) is a long outstanding problem representative of the difficulties inherent in the nonperturbative study of field theories. At present one of the most promising and often used methods of study is the numerical evaluation of path integrals in the lattice gauge formalism [1] by Monte Carlo simulation. Despite the formidable technology which has been brought to bear the lattices involved in the largest computations are still quite modest. The complimentary method to that of path integrals is the Hamiltonian formalism either on a conventional lattice [2] or, more recently, in light-cone quantized form [3]. Here again the lattices or bases of states currently accessible is frustratingly small.

Against this background of numerical work there has been steady interest in analytic approaches to the nonperturbative study of field theories. In this category one would include (but not exhaust the list) variational approaches [4], extrapolations of the strong coupling expansion [5], the Lanczos method and variants applied in operator form [6], and the t expansion [7]. The Lanczos method in operator form and the t expansion are particularly lucid as both encapsulate the physics in the analytical calculation of Hamiltonian moments $\langle H^n \rangle$ with respect to some well chosen trial state. The t expansion has the advantage of computing in the infinite lattice limit; however, the reliability of the method is undermined to some extent by the need to extrapolate to the $t \to \infty$ limit. The Lanczos method on the other hand does not suffer from such ambiguities, being a straightforward tridiagonalization of the Hamiltonian in question.

In the numerical computation of the low-lying eigenstates of Hamiltonian matrices the Lanczos method of tridiagonalization is often employed due to its efficiency and linear memory requirements. In the case of the large lattice limit of Hamiltonian models, with S states per site, the largest possible value of N, the number of sites, will be severely limited since the basis of states grows as S^N.

The Lanczos method in operator form circumvents the storage problems associated with the increasing basis size as $N \to \infty$ by being analytic in this quantity. One accommodates arbitrarily large bases at the expense of the accuracy of the calculated eigenvalues of the system. While this tradeoff may be beneficial at some intermediate values of N the direct analytical application of the Lanczos method is of limited use for large N since, in general, the computation of large orders of $\langle H^n \rangle$, required in the calculation of larger Lanczos matrices, is difficult.

In this paper it will be demonstrated that the elements of the (tridiagonal) Lanczos matrix, α_n and β_n, for a lattice Hamiltonian admit an expansion in $1/N_p$, where N_p is the number of plaquettes in the lattice, and that the terms in this expansion appear to have a simple form in n. The dependence on the physics via the Hamiltonian moments is such that higher orders of $\langle H^n \rangle$ are only required when higher orders of the expansion are computed. Application of this expansion to the Heisenberg model gives convergence to an upper bound on the ground-state energy density as $N_p \to \infty$. Furthermore the upper bound appears to approach the true infinite lattice ground-state energy density as the expansion order is increased.

Consider a Hamiltonian H defined on a lattice of N_p plaquettes. Starting with a trial state $|v_1\rangle$ one obtains a basis $\{|v_n\rangle\}$ in which H is tridiagonal, 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 the elements of the Lanczos tridiagonal matrix α_n and β_n are given by

$$\begin{aligned} \alpha_n &= \langle v_n | H | v_n \rangle , \\ \beta_n &= \langle v_{n+1} | H | v_n \rangle . \end{aligned} \tag{2}$$

In practice the full construction of the basis $\{|v_n\rangle\}$ is not required if one is interested only in the low-lying states of the system since the eigenvalues of the tridiagonal Lanczos matrix rapidly converge to those of H as the construction proceeds.

From (1) it can be seen by inspection that the Lanczos

matrix elements α_n and β_n can be written solely in terms of moments of the Hamiltonian with respect to $|v_1\rangle$, i.e.,

$$\begin{aligned}\alpha_n &= \alpha_n(\langle H\rangle, \langle H^2\rangle, \ldots, \langle H^{2n-1}\rangle)\ , \\ \beta_n &= \beta_n(\langle H\rangle, \langle H^2\rangle, \ldots, \langle H^{2n}\rangle)\ .\end{aligned} \tag{3}$$

Instead of writing the Lanczos matrix in terms of $\langle H^n\rangle$ it is convenient to use *connected* Hamiltonian moments $\langle H^n\rangle_c$ which scale with the volume as N_p. The connected moments are related to $\langle H^n\rangle$ by [7]

$$\langle H^n\rangle_c = \langle H^n\rangle - \sum_{p=0}^{n-2} \binom{n-1}{p} \langle H^{p+1}\rangle_c \langle H^{n-1-p}\rangle\ . \tag{4}$$

The N_p dependence is made explicit by defining c_n as

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

It is a straightforward task (though increasingly tedious) to calculate α_n and β_n in terms of c_n and N_p. For the first few α_n and β_n (for brevity only the 3×3 matrix is listed here) we find

$$\begin{aligned}\alpha_1 &= c_1 N_p\ , \\ \alpha_2 &= \frac{N_p c_1 c_2 + c_3}{c_2}\ , \\ \alpha_3 &= \frac{2N_p^2 c_1 c_2^4 + 4N_p c_2^3 c_3 - N_p c_1 c_2 c_3^2 + c_3^3 + N_p c_1 c_2^2 c_4 - 2c_2 c_3 c_4 + c_2^2 c_5}{c_2(2N_p c_2^3 - c_3^2 + c_2 c_4)}\ , \\ \beta_1^2 &= c_2 N_p\ , \\ \beta_2^2 &= \frac{2N_p c_2^3 - c_3^2 + c_2 c_4}{c_2^2}\ .\end{aligned} \tag{6}$$

The expressions for α_n an β_n appear cumbersome; however, upon expansion in $1/N_p$ an ordered structure becomes apparent:

$$\begin{aligned}\alpha_1 &= c_1 N_p\ , \\ \alpha_2 &= c_1 N_p + \left[\frac{c_3}{c_2}\right]\ , \\ \alpha_3 &= c_1 N_p + 2\left[\frac{c_3}{c_2}\right] + \left[\frac{3c_3^3 - 4c_2 c_3 c_4 + c_2^2 c_5}{2c_2^4}\right]\frac{1}{N_p} + \cdots\ , \\ \alpha_4 &= c_1 N_p + 3\left[\frac{c_3}{c_2}\right] + 3\left[\frac{3c_3^3 - 4c_2 c_3 c_4 + c_2^2 c_5}{2c_2^4}\right]\frac{1}{N_p} + \cdots\ , \\ \alpha_5 &= c_1 N_p + 4\left[\frac{c_3}{c_2}\right] + 6\left[\frac{3c_3^3 - 4c_2 c_3 c_4 + c_2^2 c_5}{2c_2^4}\right]\frac{1}{N_p} + \cdots\ , \\ \alpha_6 &= c_1 N_p + 5\left[\frac{c_3}{c_2}\right] + 10\left[\frac{3c_3^3 - 4c_2 c_3 c_4 + c_2^2 c_5}{2c_2^4}\right]\frac{1}{N_p} + \cdots\ ;\end{aligned} \tag{7a}$$

$$\begin{aligned}\beta_1^2 &= c_2 N_p\ , \\ \beta_2^2 &= 2c_2 N_p + \left[\frac{c_2 c_4 - c_3^2}{c_2^2}\right]\ , \\ \beta_3^2 &= 3c_2 N_p + 3\left[\frac{c_2 c_4 - c_3^2}{c_2^2}\right] + \left[\frac{-12c_3^4 + 21c_2 c_3^2 c_4 - 4c_2^2 c_4^2 - 6c_2^2 c_3 c_5 + c_2^3 c_6}{2c_2^5}\right]\frac{1}{N_p} + \cdots\ , \\ \beta_4^2 &= 4c_2 N_p + 6\left[\frac{c_2 c_4 - c_3^2}{c_2^2}\right] + 4\left[\frac{-12c_3^4 + 21c_2 c_3^2 c_4 - 4c_2^2 c_4^2 - 6c_2^2 c_3 c_5 + c_2^3 c_6}{2c_2^5}\right]\frac{1}{N_p} + \cdots\ , \\ \beta_5^2 &= 5c_2 N_p + 10\left[\frac{c_2 c_4 - c_3^2}{c_2^2}\right] + 10\left[\frac{-12c_3^4 + 21c_2 c_3^2 c_4 - 4c_2^2 c_4^2 - 6c_2^2 c_3 c_5 + c_2^3 c_6}{2c_2^5}\right]\frac{1}{N_p} + \cdots\ .\end{aligned} \tag{7b}$$

The expansions (7) suggest a general form:

$$\alpha_n = c_1 N_p + (n-1)\left[\frac{c_3}{c_2}\right] + \frac{1}{2}(n-1)(n-2)\left[\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{2c_2^4}\right]\frac{1}{N_p} + \cdots ,$$
$$\beta_n^2 = nc_2N_p + \frac{1}{2}n(n-1)\left[\frac{c_2c_4 - c_3^2}{c_2^2}\right] + \frac{1}{6}n(n-1)(n-2)\left[\frac{-12c_3^4 + 21c_2c_3^2c_4 - 4c_2^2c_4^2 - 6c_2^2c_3c_5 + c_2^3c_6}{2c_2^5}\right]\frac{1}{N_p} + \cdots . \quad (8)$$

Assuming the validity of the plaquette expansions (8) for α_n and β_n^2 one can immediately write down the expanded Lanczos matrix of any order once the required c_n have been calculated. At some critical order of the Lanczos matrix the expansion will break down (for fixed N_p); one is then interested in how close to the actual spectrum the eigenvalues of the Lanczos matrix approach before the breakdown occurs. The breakdown point will depend on the model in question through the c_n.

To investigate the convergence properties of this method we apply it to the case of the one-dimensional Heisenberg model defined on a lattice of N spins ($N_p = N$). The Hamiltonian is

$$H = \sum_{i=1}^{N} \mathbf{S}(i)\cdot\mathbf{S}(i+1) , \quad (9)$$

where $\mathbf{S}(i)$ is the spin operator at the lattice site i and periodic boundary conditions [$\mathbf{S}(N+1) = \mathbf{S}(1)$] are adopted. In the infinite lattice limit the ground-state energy density E_0/N is known to be

$$\lim_{N\to\infty} \frac{E_0}{N} = -\ln 2 + \frac{1}{4} \approx -0.443\,147 . \quad (10)$$

The connected Hamiltonian moments for this model with respect to the Néel state $|v_1\rangle \equiv |\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\ldots\rangle$ have been computed [8] up to $\langle H^{17}\rangle_c$. Since for definite values of c_n the calculation of the Lanczos matrix is far less time consuming than the general case we are able to determine the plaquette expansion to $1/N_p^3$ for the Heisenberg model. We find

$$\alpha_n = -\frac{1}{4}N_p + (n-1) - (n-1)(n-2)\frac{1}{N_p} - \frac{1}{9}(n-1)(n-2)(26n-51)\frac{1}{N_p^2} - \frac{1}{9}(n-1)(n-2)(65n^2 - 309n + 423)\frac{1}{N_p^3} + \cdots ,$$
$$\beta_n^2 = \frac{n}{4}N_p - \frac{3}{4}n(n-1) + \frac{2}{3}n(n-1)(n-2)\frac{1}{N_p} + \frac{1}{9}n(n-1)(n-2)(13n-27)\frac{1}{N_p^2} + \frac{1}{45}n(n-1)(n-2)(94n^2 - 633n + 1143)\frac{1}{N_p^3} + \cdots . \quad (11)$$

Given the plaquette expansion of the Heisenberg model

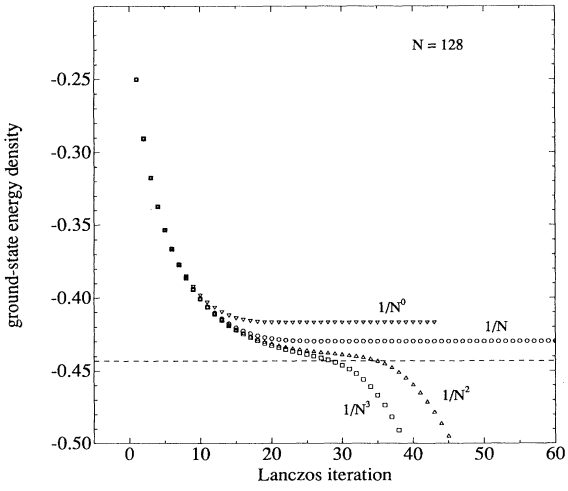

FIG. 1. The ground-state eigenvalue, $\lambda_0^{(r)}(m, N_p)/N_p$, as a function of the Lanczos matrix size (or iteration) for various expansion orders, $r = 0$ to $r = 3$, at $N_p = 128$. The dashed line is the true infinite lattice ground-state energy density.

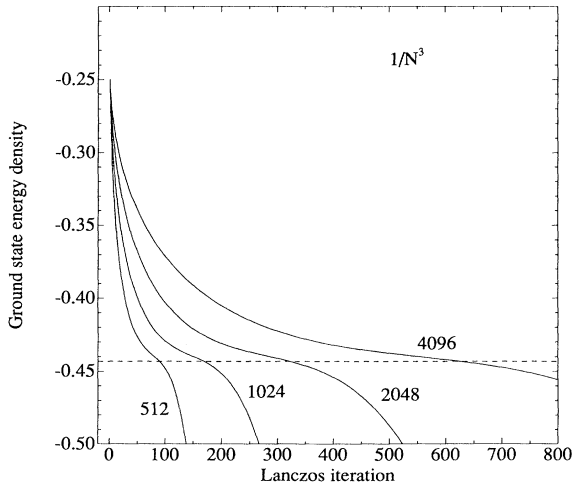

FIG. 2. Behavior of the $r = 3$ expansion for increasing lattice sizes. The dashed line is the true infinite lattice ground-state energy density.

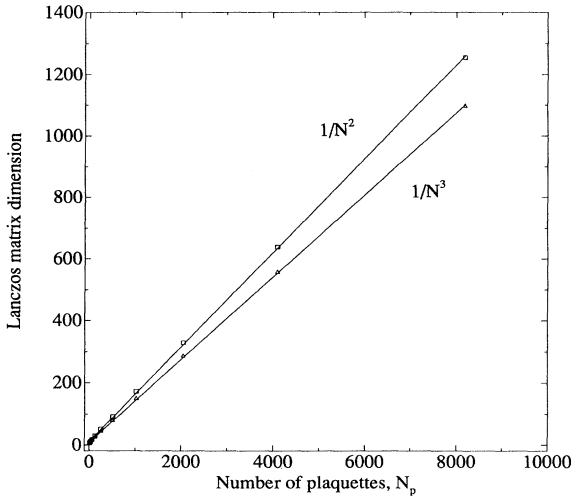

FIG. 3. Dimension of the maximum Lanczos matrix (corresponding to the point of inflection), as a function of the number of plaquettes.

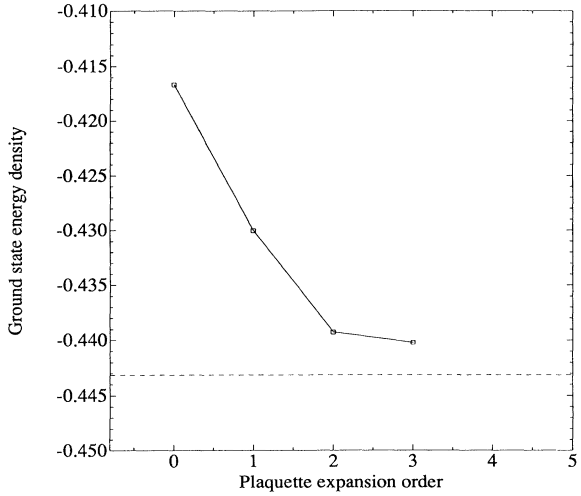

FIG. 5. The ground-state energy density $\mathcal{E}_0^{(r)}$, plotted for expansion orders $r=0$ to $r=3$.

to order $1/N_p^r$ we construct the Lanczos matrix of increasing dimension m and examine the ground-state eigenvalue $\lambda_0^{(r)}(m,N_p)$ as a function of m. In Fig. 1 the ground-state energy density $\lambda_0^{(r)}(m,N_p)/N_p$ is plotted for various expansion orders up to $1/N_p^3$ for a typical case ($N_p=128$). For both $1/N_p^0$ and $1/N_p$ expansions there is no critical point and the eigenvalue converges (for the case of $1/N_p^0$ the Lanczos procedure terminates when $\beta_n^2<0$). For higher expansion orders the expansion breaks down as one naively expects for m such that the last term in the expansion becomes significant. Figure 2 shows the point of breakdown occurring for larger values of m as the number of plaquettes is increased. The ground-state energy density evaluated just before the breakdown converges as $N_p\rightarrow\infty$. To see this we assume the Lanczos iteration corresponding to the point of inflection, m_i, to be the last true point before the breakdown occurs. The linear dependence with N_p of the maximum Lanczos matrix (i.e., that corresponding to the point of inflection) is shown in Fig. 3. Taking $\lambda_0^{(r)}(m_i,N_p)/N_p$ as the ground-state energy density corresponding to a given lattice size we see in Fig. 4 the convergence of this quantity as $N_p\rightarrow\infty$ for the different expansion orders, i.e.,

$$\lim_{N_p\rightarrow\infty}\frac{\lambda_0^{(r)}(m_i,N_p)}{N_p}=\mathcal{E}_0^{(r)}\ . \tag{12}$$

Finally we plot the infinite lattice limit of the ground-state energy density $\mathcal{E}_0^{(r)}$ for each expansion order in Fig. 5 indicating the approach to the true infinite result.

In this work it has been demonstrated that there exists a plaquette expansion of the Lanczos matrix of lattice Hamiltonian models and that its form is not only simple, but also uniform for all models; the physics enters solely via the connected Hamiltonian moments. The plaquette expansion allows one to write down the Hamiltonian in tridiagonal basis to a given order in $1/N_p$ immediately once the required connected Hamiltonian moments have been calculated. Working in the Heisenberg model it was shown that the ground-state energy density obtained from the plaquette expansion approaches the infinite lattice result. If this phenomenon holds in general then the plaquette expansion may be useful in the calculation of the spectrum of various models in the infinite lattice limit, particularly since the amount of computational work once the Hamiltonian moments have been calculated is minimal. It still remains, however, to prove that the plaquette expansion to any given order in $1/N_p$ is valid to all orders in the Lanczos matrix.

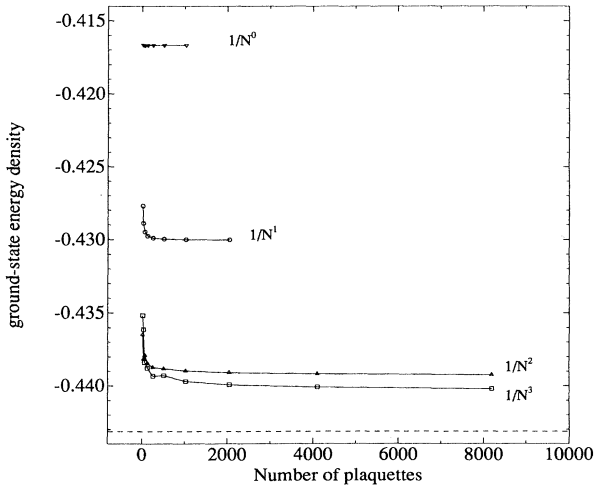

FIG. 4. Convergence properties of the quantity $\lambda_0^{(r)}(m_i,N_p)/N_p$ as $N_p\rightarrow\infty$. The dashed line is the true infinite lattice ground-state energy density.

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