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Staggered Magnetisation in the Heisenberg Antiferromagnet

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Abstract

In the presence of a staggered magnetic field, the plaquette expansion of the Lanczos matrix elements are obtained for the antiferromagnetic 2D Heisenberg model up to order $1/N_p$ (N_p is the number of plaquettes on the lattice). The resulting approximate tri-diagonal form of the Hamiltonian is diagonalised for various values of the field strength in the $N_p \to \infty$ limit for the ground state energy density. From the behaviour of the ground-state energy density at weak fields, the staggered magnetisation at this order in the plaquette expansion is found to be $0 \cdot 71$ (in units where the Néel state staggered magnetisation is $1 \cdot 0$).

1. Introduction

The two-dimensional antiferromagnetic Heisenberg model has been the subject of a great deal of work over the past few years in connection with the undoped copper oxides (Manousakis 1991). Unlike the one-dimensional case, the model has not been solved exactly, instead the ground state properties have been studied numerically for the most part. Techniques such as Monte Carlo, series, direct diagonalisation and spin-wave theory have been employed in the calculation of ground state properties in the bulk limit. Whilst the ground state energy is now known to high precision (Manousakis 1991; Weihong *et al.* 1991; Runge 1992), the staggered magnetisation, an indication of the degree of order in the ground state, is not known as accurately—although results consistently suggest the existence of long range antiferromagnetic order.

Most methods usually involve calculating quantities on finite lattices and extrapolating to the bulk limit. A new many-body technique, the plaquette expansion (Hollenberg 1993*a*), which calculates directly in the bulk limit without extrapolation, has recently been applied to the two-dimensional antiferromagnetic Heisenberg model with quite satisfactory results for the ground state energy density (Tomlinson and Hollenberg 1993). This calculation was primarily a study of the method itself, using the precision of the ground state energy density for this model as a guide. The plaquette expansion is a cluster expansion of the Lanczos tri-diagonal matrix elements in terms of the number of plaquettes N_p. In this paper we extend these calculations to that of the ground state staggered magnetisation by calculation of the ground state energy in the presence of a staggered magnetic field.

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The paper is organised as follows. In Section 2 the plaquette expansion method is outlined. In Section 3 results for the application of the method to the 2D Heisenberg antiferromagnet in a staggered magnetic field are given and the staggered magnetisation is calculated.

2. The Plaquette Expansion

For 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. An expansion in the number of plaquettes on the lattice leads to the following forms for α_n and β_n:

$$\alpha_n = N_p c_1 + (n-1)\frac{c_3}{c_2} + \tfrac{1}{2}(n-1)(n-2)\frac{3c_3^3 - 4c_2c_3c_4 + c_2^2c_5}{2c_2^4}\frac{1}{N_p} + \dots\,,$$

$$\beta_n^2 = nc_2N_p + \tfrac{1}{2}n(n-1)\frac{c_2c_4 - c_3^2}{c_2^2}$$

$$+\tfrac{1}{6}n(n-1)(n-2)\frac{-12c_3^4 + 21c_2c_3^2c_4 - 4c_2^2c_4^2 - 6c_2^2c_3c_5 + c_2^3c_6}{2c_2^5}\frac{1}{N_p} + \dots\,, \tag{2}$$

where the connected coefficients are defined in terms of the connected Hamiltonian moments as $\langle H^n\rangle_c \equiv c_nN_p$. The first two terms of the above expansions have been rigorously established (Witte and Hollenberg 1993); whilst the proof for the higher order terms is straightforward, the amount of algebra involved has prevented it being carried out to higher order. However, the above expressions have been verified to the ninth Lanczos iteration by direct calculation in the one-dimensional Heisenberg model (Hollenberg 1993*b*).

The plaquette expansion is completely general. The only difference in application to various models are the connected coefficients c_n. The connected moments of the Hamiltonian are calculated with respect to a trial state chosen in the appropriate sector of Hilbert space. After constructing the set of tri-diagonal Lanczos matrices corresponding to plaquette expansions of α_n and β_n to order $1/N_p^r$, one examines the eigenvalue of interest, in this case the lowest eigenvalue $\lambda_0^{(r)}(N_p,l)$, as a function of the Lanczos iteration l. Defining the ground state energy $E_0^{(r)}(N_p)$, given by the converged value of the eigenvalue $\lambda_0^{(r)}(N_p,l)$, one can take the limit $N_p\to\infty$, i.e.

$$\lim_{N_p\to\infty}\frac{E_0^{(r)}(N_p)}{N_p} = \mathcal{E}_0^{(r)}\,. \tag{3}$$

The zero-field result for the energy density $\mathcal{E}_0^{(1)}$ of the 2D Heisenberg antiferromagnet was found to be within $0\cdot8\%$ of the exact result (Tomlinson and Hollenberg 1993) and serves as an indication of the accuracy of the calculations presented here.

3. The 2D Heisenberg Model in a Staggered Field

The Hamiltonian of the antiferromagnetic Heisenberg model in two dimensions on a periodic square lattice of N spins ($N_p = N$) is given by

$$H = \sum_{\langle i,j \rangle} \vec{S}_i \, . \, \vec{S}_j \; + \; 2B \sum_i \zeta_i S_i^z \, , \tag{4}$$

where B is the magnetic field and $\zeta_i = \pm 1$ alternates on the two sublattices. The staggered magnetisation M is the expectation value of the field term in the ground state,

$$M \equiv \lim_{B \to 0} \lim_{N_p \to \infty} \langle \psi_{g.s.} | \frac{1}{N_p} \sum_i \zeta_i S_i^z | \psi_{g.s.} \rangle \, . \tag{5}$$

In this notation the Néel state has staggered magnetisation $M_{\text{Néel}} = 1$.

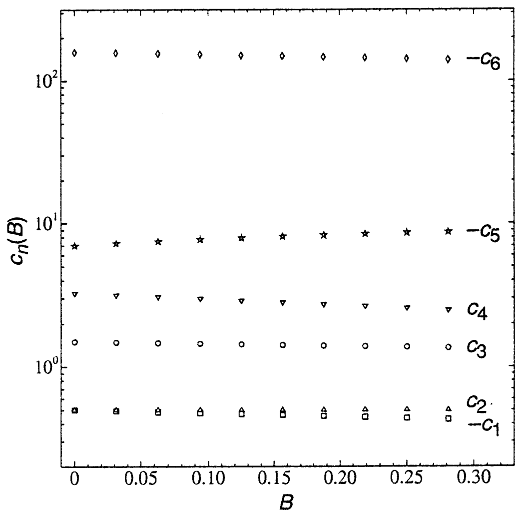


Fig. 1. Connected Hamiltonian moments $c_n(B)$ with respect to the Néel state for various values of the field B.

To obtain the plaquette expansion we calculate the connected Hamiltonian moments $c_n(B)$ with respect to the Néel state for various values of the field B. The $c_n(B)$ are shown in Fig. 1. These connected moments form the basis of the plaquette expansion for each value of B. In Fig. 2 the lowest eigenvalue of the Lanczos matrix contructed from the $r = 0, 1$ plaquette expansions for α_n and β_n is shown for representative values of B. In the case of the $r = 0$ expansion there is convergence for all B. The $r = 1$ expansion develops an inflection as B is increased; the converged value is taken at the minimum slope. This convergence region flattens as $N_p \to \infty$ and the energy density $E_0^{(1)}(N_p)/N_p$ converges in the bulk limit as shown in Fig. 3. The energy densities $\mathcal{E}_0^{(0)}(B)$ and $\mathcal{E}_0^{(1)}(B)$ are calculated for each value of B and plotted in Fig. 4.

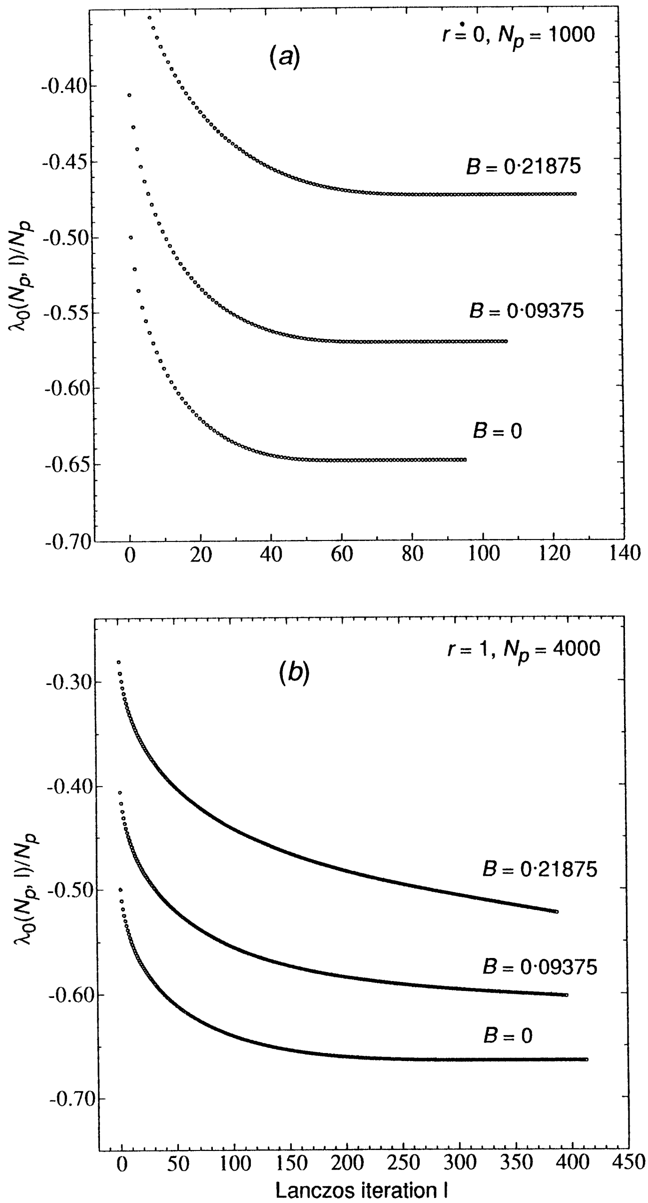
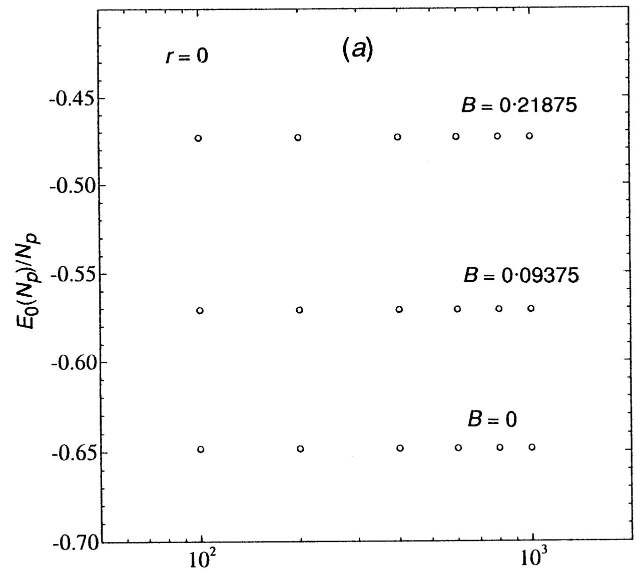


Fig. 2. Ground state eigenvalue $\lambda_0^{(r)}(N_p, l)$ as a function of Lanczos iteration l for (a) $r = 0$ ($N_p = 1000$) and (b) $r = 1$ ($N_p = 4000$) expansions.

From the slopes of these lines near $B = 0$ we find the staggered magnetisation for the $r = 0, 1$ plaquette expansions to be

$$M^{(0)} = 0{\cdot}84\,, \qquad M^{(1)} = 0{\cdot}71\,. \tag{6}$$



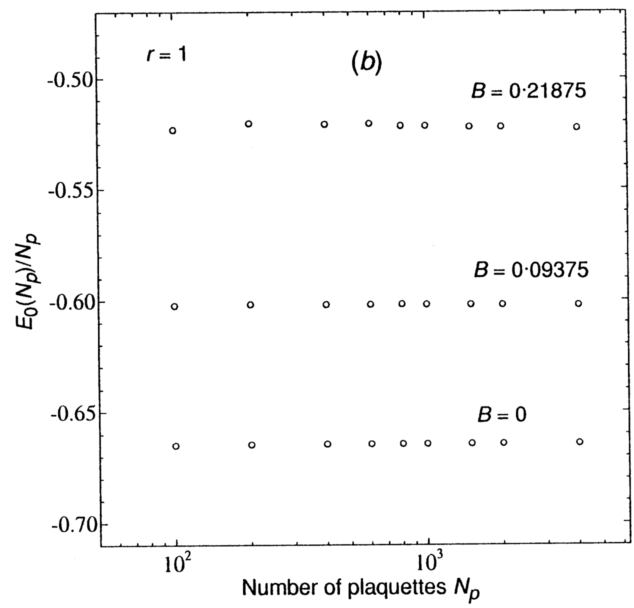


Fig. 3. Ground state energy density, $E_0^{(r)}(N_p)/N_p$, in the large-lattice limit, $N_p \to \infty$, for (a) $r = 0$ and (b) $r = 1$ expansions.

From a critical survey of the literature, Manousakis (1991) estimated the staggered magnetisation to be in the range $0{\cdot}62 \pm 0{\cdot}04$. This is based on agreement between various Monte Carlo calculations (Runge 1992; Trevedi and Ceperly 1989; Reger and Young 1988; Gross *et al.* 1989), series expansions (Weihong *et al.* 1991) and spin-wave theory. The plaquette expansion result $M^{(1)}$ is a significant improvement over the first-order result $M^{(0)}$ and agrees

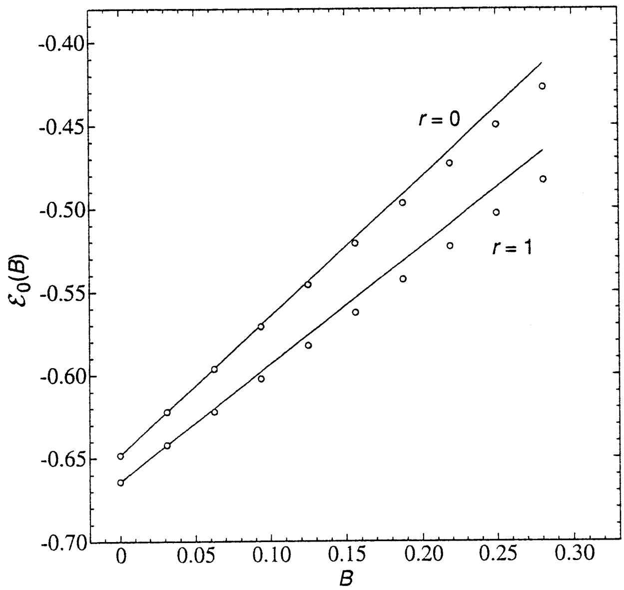


Fig. 4. Bulk-limit ground state energy density, $\mathcal{E}_0^{(r)}(B)$ $(r = 0, 1)$, as a function of the field B.

reasonably well with this consensus. Since for weak fields one would expect the overlap with the Néel state to still be significant, the energy density $\mathcal{E}_0^{(1)}(B)$ should be of a similar precision to the zero-field case. This would imply that the precision of the staggered magnetisation derived here is of the order of a few per cent. However, in comparison with other calculations the precision is at the 10% level. Although this method has the advantage of computing directly in the infinite-lattice limit, at low order in the expansion finite-cluster effects will affect the results. We see the first-order plaquette expansion result has quite a high value of this order parameter, whilst at the next order this is decreased somewhat as the increase in cluster size allows for a greater effect of the quantum fluctuations on the long-range order.

Clearly, the staggered magnetisation is more sensitive to the cluster size than the ground state energy density. However, the plaquette expansion is still a promising method of calculating such order parameters. Eventually the cluster size should saturate the quantum fluctuations against long-range order and hence such calculations carried to higher order may eventually give a stable result for the staggered magnetisation in the infinite-lattice limit.

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References

Gross, M., Sanchez-Velasco, E., and Siggia, E. (1989). *Phys. Rev.* B **39**, 2484.
Hollenberg, L. C. L. (1993*a*). *Phys. Rev.* D **47**, 1640.
Hollenberg, L. C. L. (1993*b*). *Phys. Lett.* A **182**, 238.

Manousakis, E. (1991). *Rev. Mod. Phys.* **63**, 1.
Reger, J. D., and Young, A. P. (1988). *Phys. Rev.* B **37**, 5978.
Runge, K. J. (1992). *Phys. Rev.* B **45**, 12292.
Tomlinson, M. J., and Hollenberg, L. C. L. (1993). 'Plaquette expansion of the 2D antiferromagnetic Heisenberg model', Preprint UMP-93–09.
Trevedi, N., and Ceperly, D. M. (1989). *Phys. Rev.* B **40**, 2737.
Weihong, Z., Oitmaa, J., and Hamer, C. J. (1991). *Phys. Rev.* B **43**, 8321.
Witte, N. S., and Hollenberg, L. C. L. (1993). 'Plaquette expansion proof and interpretation', Preprint UMP-93–87.

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