J_1-J_2 model: Energy, correlations, and order-parameter fluctuations on finite lattices

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A modified spin-wave theory is applied to frustrated quantum antiferromagnets on finite square lattices. The results for the energy and for the correlation functions are found to agree very well with exact values obtained by numerical methods. The fluctuations of different order parameters, previously proposed to characterize possible different phases of purely quantum origin, are investigated. Our results suggest that the enhancement of long-range dimer and twist order seen numerically is not significant, and is due to the finite size of the lattices considered.

The Cu-O planes in undoped high-T_c compounds are well described[1] by a square-lattice Heisenberg model displaying[2] long-range antiferromagnetic order. Upon doping, this long-range order is destroyed[3] and a different nonmagnetic phase sets in, the fluctuations of which are believed[4] to be central to a microscopic understanding of the high-T_c phenomena. Following the suggestion[5] that the effect of holes in destroying the Néel order can be accounted for by the introduction of frustration in the original Heisenberg model, many authors[6-9] considered the possibility of finding such phases in frustrated quantum antiferromagnets. In this regard the simplest model one can think of is the so-called J_1-J_2 model:

$$H = J_1 \sum_{i,\delta} \mathbf{S}_i \cdot \mathbf{S}_{i+\delta} + J_2 \sum_{i,\delta'} \mathbf{S}_i \cdot \mathbf{S}_{i+\delta'} , \quad (1)$$

which includes, in addition to the standard J_1 Heisenberg coupling, a frustrating next-nearest-neighbor interaction J_2 along the diagonal δ' of the square-lattice plaquettes. Classically, the ground state of this model has Néel order for $J_2/J_1 < 0.5$, while for $J_2/J_1 > 0.5$ it decouples into two Néel sublattices with an energy independent of the angle between the corresponding staggered magnetizations. At $J_2/J_1 = 0.5$ various states become degenerate, suggesting that near this point quantum fluctuations could stabilize a new phase with some kind of disorder. The nature of this phase is of considerable interest, and several candidates for the ground state in the intermediate-parameter region near $J_2/J_1 = 0.5$ have been proposed: resonant-valence-bond state with short-range order,[6] long-range dimer order in a columnar pattern,[8] twist order,[9] and the more exotic chiral order.[10] Most of the proposals come from studies involving approximations such as conventional (large-S) spin-wave theory or a variety of mean-field decouplings, which disregard, in one way or another, part of the fluctuations originating in the quantum nature of the spins. Consequently, more reliable techniques are needed to establish faithfully the existence of any of these states of purely quantum origin. One alternative is provided by numerical methods—mainly exact diagonalization of small systems—although in this case it is hard to extrapolate the results to the infinite-size limit (see note added).

Clearly, it would be desirable to have analytical approximations capable of providing a bridge between the exact, small-system results and the unreliable, infinite-size approximations, that is, a method which could reproduce—at least qualitatively—the results obtained for finite systems, while having a well-defined behavior with lattice size. Takahashi[11] has recently formulated a constrained spin-wave theory (SWT) of the unfrustrated Heisenberg model, which yields excellent agreement with the results of exact diagonalization for small systems (even the exact results for the smallest lattices[12]). His idea was to supplement the conventional SWT with the condition of zero magnetization for low-dimensional systems at finite temperatures (Mermin-Wagner theorem) and for finite systems at $T = 0$.[12] This is implemented by means of a constraint introduced through a Lagrange multiplier, which acts as a chemical potential for spin-wave bosons. Since, for the unfrustrated Heisenberg model, successful extrapolations of finite-size results use SWT as a guide,[2] Takahashi's theory works well as the bridge approximation we were claiming for above. Unfortunately, attempts to use it for the J_1-J_2 model showed that the results deteriorate rapidly with the amount of frustration introduced.[13]

More recently, Xu and Ting[14] have generalized this theory by dressing the excitations through the self-consistent decoupling of quartic interactions in the spin-wave Hamiltonian. The renormalized phase diagram they obtained for the J_1-J_2 model differs qualitatively from that obtained with conventional theory.[6] In particular, they found no windows in the intermediate-parameter region between the two classical magnetic phases of the model, suggesting the existence of a new phase, different from the spin-liquid state proposed in earlier studies.[6] Since their results for $N \to \infty$ come close to those obtained by numerical methods,[7] it seems to us that this approximation deserves a better look at its predictions, particularly on finite lattices.

In this work we investigate how well the constrained self-consistent SWT reproduces the exact results obtained in numerical studies of the J_1-J_2 model.[7,13] Conversely, by reproducing qualitatively results obtained for finite systems, we will try to assess whether some features

found numerically are significant or only due to the finite size of the lattices considered. To this end we compute four-spin correlation functions, which are needed to study the fluctuations of different order parameters as a function of lattice size. These order parameters have been previously proposed in the literature in order to characterize the nature of (possible) new phases in the intermediate-parameter region. Since our interest is focused on ground-state properties, all the calculations will be carried out at zero temperature.

Following Takahashi,[11] we add to Hamiltonian (1) the constraint of zero total (staggered) magnetization,

$$H'=H+\lambda\sum_i(-1)^i S_i^z ,$$

where $(-1)^i=1$ (-1) for spins pointing up (down) in the classical ground state. A standard Dyson-Maleev transformation[15] of spin operators in H' leaves us with a spin-wave Hamiltonian in Bose operators with quartic interactions. Further Hartree-Fock decoupling of these quartic terms, plus a Bogoliubov diagonalization of the resulting quadratic Hamiltonian, produced the following results.

(a) Néel phase ($J_2/J_1<0.5$),

$$\left\langle\frac{H'}{2N}\right\rangle=J_1\langle\mathbf{S}_i\cdot\mathbf{S}_{i+\delta}\rangle+J_2\langle\mathbf{S}_i\cdot\mathbf{S}_{i+\delta'}\rangle$$
$$=-J_1[g(\delta)]^2+J_2[f(\delta')]^2 , \quad (2)$$

where

$$g(\mathbf{r})=\frac{1}{2N}\sum_{\mathbf{k}}\frac{\eta_{\mathbf{k}}\gamma_{\mathbf{k}}}{(1-\eta_{\mathbf{k}}^2\gamma_{\mathbf{k}}^2)^{1/2}}e^{i\mathbf{k}\cdot\mathbf{r}} , \quad (3a)$$

$$f(\mathbf{r})=\frac{1}{2N}\sum_{\mathbf{k}}\frac{1}{(1-\eta_{\mathbf{k}}^2\gamma_{\mathbf{k}}^2)^{1/2}}e^{i\mathbf{k}\cdot\mathbf{r}} , \quad (3b)$$

$$\eta_{\mathbf{k}}=\eta\left[1-\frac{J_2 g(\delta_x)}{J_1 f(\delta_y)}\eta(1-\gamma'_{\mathbf{k}})\right]^{-1} , \quad (3c)$$

and $\gamma_{\mathbf{k}}=\frac{1}{2}(\cos k_x+\cos k_y)$, $\gamma'_{\mathbf{k}}=\cos k_x\cos k_y$, and $\eta=[1-\lambda/J_1 z g(\delta)]^{-1}$.

(b) Collinear phase[16] ($J_2/J_1>0.5$),

$$\left\langle\frac{H'}{2N}\right\rangle=J_1\langle\mathbf{S}_i\cdot\mathbf{S}_{i+\delta_x}\rangle+J_1\langle\mathbf{S}_i\cdot\mathbf{S}_{i+\delta_y}\rangle+2J_2\langle\mathbf{S}_i\cdot\mathbf{S}_{i+\delta'}\rangle$$
$$=-J_1[g(\delta_x)]^2+J_1[f(\delta_y)]^2-2J_2[g(\delta')]^2 , \quad (4)$$

where, in this case,

$$g(\mathbf{r})=\frac{1}{2N}\sum_{\mathbf{k}}\frac{A_{\mathbf{k}}}{(B_{\mathbf{k}}^2-A_{\mathbf{k}}^2)^{1/2}}e^{i\mathbf{k}\cdot\mathbf{r}} , \quad (5a)$$

$$f(\mathbf{r})=\frac{1}{2N}\sum_{\mathbf{k}}\frac{B_{\mathbf{k}}}{(B_{\mathbf{k}}^2-A_{\mathbf{k}}^2)^{1/2}}e^{i\mathbf{k}\cdot\mathbf{r}} , \quad (5b)$$

and

$$A_{\mathbf{k}}=\frac{g(\delta_x)}{f(\delta_y)}\cos k_x+\frac{2J_2 g(\delta')}{J_1 f(\delta_y)}\gamma'_{\mathbf{k}} ,$$

$$B_{\mathbf{k}}=\frac{g(\delta_x)}{f(\delta_y)}-1+\cos k_y+\frac{2J_2 g(\delta')}{J_1 f(\delta_y)}-\frac{\lambda}{2J_1 f(\delta_y)} .$$

In both phases the consistency equations (3) and (5) must be supplemented by the zero-magnetization condition $f(0)=S+\frac{1}{2}$, imposed through the Lagrange multiplier.

In the thermodynamic limit $N\to\infty$ and for λ equal to zero, these equations reduce to the Xu-Ting equations[14] (in this limit the system does get magnetized so that the Lagrange multiplier that ensures zero magnetization must vanish). Note also that when $\lambda=0$ there are divergent terms in the k summations for $\mathbf{k}=0,\pi$, which have to be treated like in the Bose-condensation problem.[17] The point $J_2/J_1=0.5$ is the classical phase boundary separating the Néel and collinear orders for $S\to\infty$. For $S=\frac{1}{2}$ there is a strong renormalization of the phase diagram because of quantum fluctuations, leaving a region of coexistence of both orders where presumably a new phase sets in.[14]

We have numerically evaluated Eqs. (2)–(5) for finite lattices. In Fig. 1 we plot the predictions for the energy of systems of sizes $N=16$ and 20, together with the exact results from Ref. 7. As can be seen, for $N=20$ our results are in very good agreement with the exact ones in both phases and in the whole parameter region; for $N=16$ the approximation does not follow the rounded shape of the exact curve near the transition point (a consequence of the absence of level crossing for this lattice[7]). Of course, for finite systems we do not expect the breaking of lattice-rotation symmetry implied by collinear order. Nevertheless, the energy in this phase is surprisingly well approximated by taking the symmetry-broken state as starting point in the calculation.

The results for correlation functions and structure factor in the Néel phase are shown in Figs. 2 and 3, where we also plot the exact results taken from Ref. 13 for comparison. Again, the agreement is excellent in the whole region corresponding to this phase, except for $N=16$, where the additional symmetries of this lattice

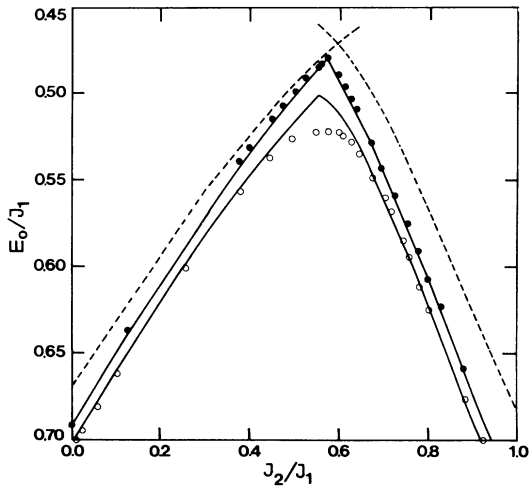
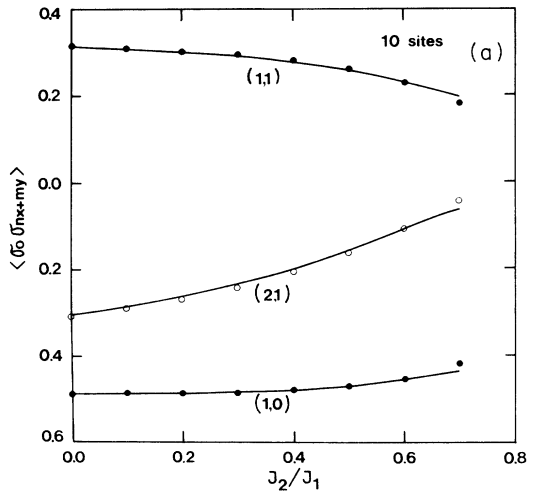
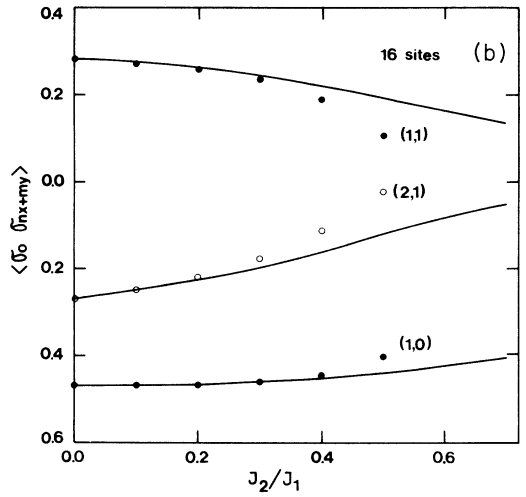


FIG. 1. Ground-state energy per bond for $N=16$ (lower solid line), $N=20$ (upper solid line), and $N=\infty$ (dashed line). Also shown are exact results for $N=16$ (open circles) and $N=20$ (solid circles) from Ref. 7.





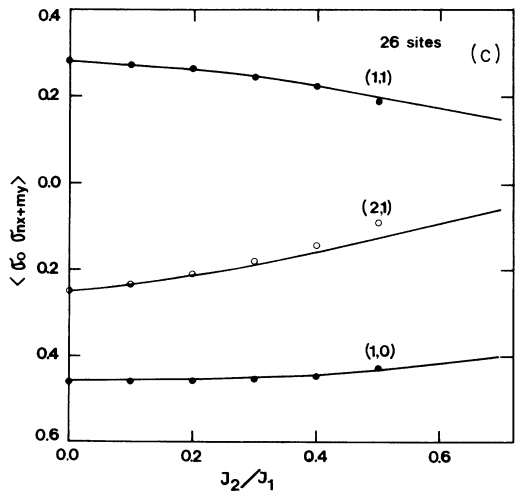


FIG. 2. Correlation functions $\langle \sigma_0 \sigma_r \rangle \equiv \frac{4}{3} \langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle$, with $\mathbf{r} = n\hat{\mathbf{x}} + m\hat{\mathbf{y}}$ for different lattice sizes: (a) $N = 10$, (b) $N = 16$, and (c) $N = 26$. Circles are exact values from Ref. 13.

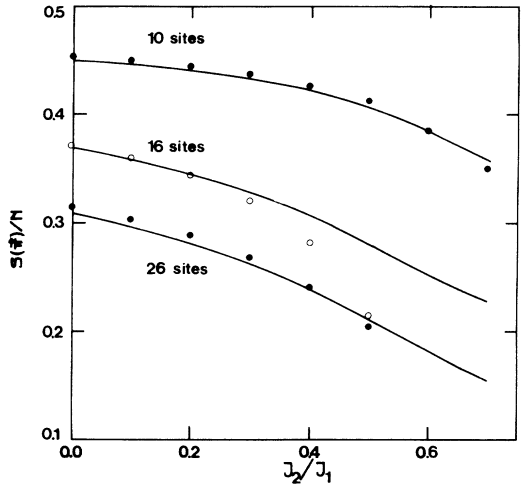


FIG. 3. Rotationally averaged structure factor per site for different lattice sizes. Circles are exact values from Ref. 13.

produce a nonsystematic behavior not mimicked by the approximation.

In order to check whether or not the constrained self-consistent SWT can reproduce more subtle quantities, we have also evaluated the four-spin correlation functions. The calculation involves pairing several eight-operator terms, producing finally expressions with a few dozen terms, which will not be reproduced here. The knowledge of the four-spin correlations allows us to study the fluctuations of different order parameters on finite lattices, which in turn provides information on lattice-size behavior of peaks or enhancements observed in numerical studies.[7]

We have considered the fluctuations in the Néel phase of the following order parameters:

$$O_{\text{Néel}} = \frac{1}{N} \sum_{\mathbf{r}} (-1)^{x+y} S^z_{\mathbf{r}}, \quad \mathbf{r} = (x,y) ,$$

$$O_{\text{collinear}} = \frac{1}{N} \sum_i \mathbf{S}_i \cdot (\mathbf{S}_{i+\hat{x}} + \mathbf{S}_{i-\hat{x}} - \mathbf{S}_{i+\hat{y}} - \mathbf{S}_{i-\hat{y}}) ,$$

$$O_{\text{column}} = \frac{1}{N} \sum_i \eta(i) \mathbf{S}_i \cdot (\mathbf{S}_{i+\hat{x}} + i\mathbf{S}_{i+\hat{y}} - \mathbf{S}_{i-\hat{x}} - i\mathbf{S}_{i-\hat{y}}) ,$$

$$O_{\text{twist}} = \frac{1}{N} \sum_i \mathbf{S}_i \times (\mathbf{S}_{i+\hat{x}} + \mathbf{S}_{i+\hat{y}}) ,$$

where i are even sites and $\eta(i) = 1$ (-1) if both i_x and i_y are even (odd).

The susceptibility of the Néel order parameter is essentially the structure factor $S(\pi,\pi)$, so that its calculation does not require the four-spin correlations. It was already plotted in Fig. 3 for $N = 10, 16, 26$; for $N = 20$ it is shown in Fig. 4 together with the susceptibility of the collinear order parameter. For this lattice size the results for $\chi_{\text{Néel}}$ agree very well up to the classical transition point $J_2/J_1 = 0.5$; for $0.5 < J_2/J_1 \leq 0.6$ (where we approximately enter the collinear phase), the approximation overestimates the exact values. In fact, this is the parameter region where a new phase is more likely to be

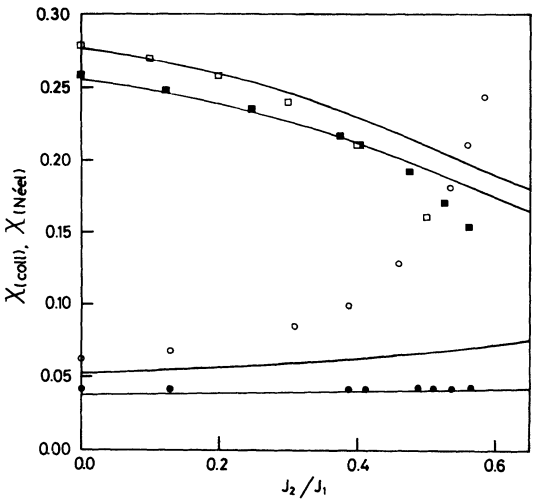


FIG. 4. Néel and collinear order-parameter susceptibilities. Open (solid) circles are exact results for $N=16$ (20) from Ref. 7.

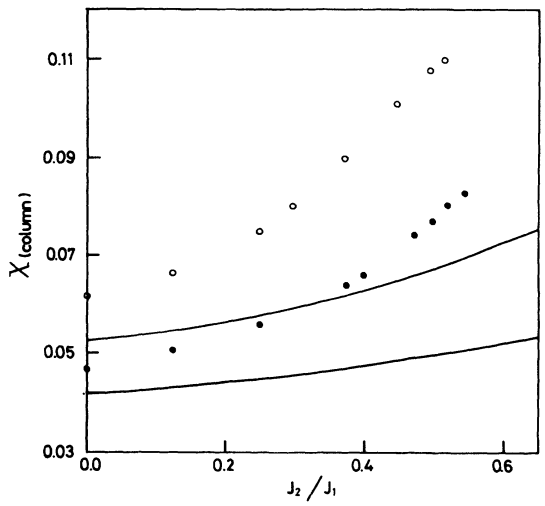


FIG. 5. Column order-parameter susceptibility. Open (solid) circles are exact results for $N=16$ (20) from Ref. 7.

present, the strongest candidate being the dimer order in a columnar pattern[8] (see below). The predicted $\chi_{\text{collinear}}$ values are very small in the whole Néel phase, as expected, and in remarkably good agreement with the exact ones. Results for $N=16$ are also included in Fig. 4 for comparison. Note the early enhancement of collinear order shown by the exact results and the large departure of approximated values from exact ones for this particular lattice.

Probably, the most interesting quantity is the column order-parameter susceptibility, whose behavior is plotted in Fig. 5. In this case the results are not very good quantitatively, but still not too far from the exact ones, and show the qualitative behavior seen numerically.[7] This is in part satisfactory since χ_{column} takes very small values (compared with the maximum possible ones), which result from subtle cancellations among four-spin correlations (one must bear in mind that we are reproducing the behavior of a parameter associated with a nonmagnetic phase, by means of an approximation which essentially relies on having a magnetized ground state). In any case, were we going to trust this result, since the curve flattens to zero for $N\rightarrow\infty$, it would mean that columnar order is not present in the thermodynamic limit.

We have also computed the susceptibility of the twist order parameter. However, in this case the results are quantitatively wrong, even unphysical (negatives) for small J_2. The reason for this can be understood as follows. Consider four spins 1,2,3,4 with 1,3 in sublattice A and 2,4 in sublattice B. By means of the Lagrange identity, it can be seen that χ_{twist} is a summation over ground-state averages such as

$$\langle(\mathbf{S}_1\cdot\mathbf{S}_3)(\mathbf{S}_2\cdot\mathbf{S}_4)\rangle-\langle(\mathbf{S}_1\cdot\mathbf{S}_2)(\mathbf{S}_3\cdot\mathbf{S}_4)\rangle\ .$$

Exact calculations on a 2×2 lattice show that our approximation gives good results for $\langle(\mathbf{S}_1\cdot\mathbf{S}_3)(\mathbf{S}_2\cdot\mathbf{S}_4)\rangle$ (in fact, the exact value 0.0625 for $J_2=0$), while it largely overestimates correlations of the type $\langle(\mathbf{S}_1\cdot\mathbf{S}_2)(\mathbf{S}_3\cdot\mathbf{S}_4)\rangle$ (exact value 0.25 for $J_2=0$ against a prediction of 0.337). Since this last type of correlation appears always with negative sign in χ_{twist}, the cancellations which take place in χ_{column} do not occur in this case, producing the above-mentioned negative results for small J_2. Nevertheless, it is interesting to comment that, for large J_2, χ_{twist} grows in going from $N=16$ to 20 (as in the numerical study[7]) and later decreases to zero for larger lattices. Were this qualitative behavior to be trusted, we would conclude that the enhancement of twist order seen numerically is only a consequence of the particular lattice sizes considered.

In conclusion, the constrained self-consistent SWT gives very good results on finite lattices for energy (in both phases) and correlation functions in the Néel phase for $J_2/J_1\leq0.5$. In the intermediate-parameter region $0.5<J_2/J_1\leq0.6$, its predictions for correlation functions and structure factor depart from the exact values, leaving open the possibility of a new phase very close in energy to the Néel state. In order to have a deeper check on the theory, we have also computed four-spin correlations. It turns out to be that at least half of these functions are inaccurately given by the approximation, which is not unexpected since four-body operators are most of the time out of reach of simple Hartree-Fock-like theories. Nevertheless, calculations of different order-parameter susceptibilities by means of this four-spin correlation produced results in good quantitative (for $\chi_{\text{collinear}}$) or qualitative agreement with exact ones. Since order parameters are carefully chosen to distinguish a Néel-like ground state from other possibilities, our results suggest that peaks or enhancements seen in numerical studies mean no more than the following: When on finite lattices the precursor Néel order is fading away as a result of frustration, all these parameters tend to fluctuate a little more, even though they will not eventually become the new ground state in the thermodynamic limit. This is seen in our calculations, where we found order-parameter enhancements in a region which, according to the same approximation, will clearly display weak Néel order for

$N \to \infty$. Finally, it would be interesting to perform similar calculations at finite temperature in order to make a comparison with a recent numerical study[18] of the thermodynamics of the model on a 4×4 lattice.

We have recently become aware of recent work by H. J. Schulz and T. A. L. Ziman where they numerically diagonalize a 6×6 lattice and make a finite-size scaling study using the 4×4 and 6×6 lattice results. Their findings, as ours, hint at a strong finite-size dependence of relevant quantities.

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