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LETTER TO THE EDITOR

A modified Holstein–Primakoff approach to frustrated quantum spin systems

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Abstract. A simple modification of conventional spin-wave theory based on the Holstein–Primakoff transformation is investigated. On the basis of a comparison with exact results on finite lattices it is shown to give substantially improved results, especially for highly frustrated systems.

The spin-wave approximation [1] is one of the oldest and simplest approaches to the physics of quantum spin systems. Recently several papers [2–5] have dealt with a modification of this approximation that makes it surprisingly good when compared with other methods and exact results. As formulated by Takahashi [2], the strategy is to supplement the usual spin-wave theory (SWT) by adding the constraint that the density of spin waves is equal to the quantum spin number S. This restriction takes into account as an average the so-called kinematical interaction: the number of bosons per site cannot exceed $2S$. Stated differently, it enforces the constraint of zero total (staggered) magnetization for (anti-) ferromagnetic spin systems on finite lattices [4].

One problem with Takahashi's theory is that it is not rotationally invariant: the constraint has to be imposed by means of a Lagrange multiplier, which is equivalent to adding an external field to the spin system. Consequently, rotationally invariant quantities must be averaged on an *ad hoc* fashion to get meaningful results. On the other hand, ignoring kinematical interactions is not the only approximation one makes in conventional SWT. For instance, when using Holstein–Primakoff transformation [6], square root operators $(1 - a^\dagger a/2S)^{1/2}$ must be expanded keeping only the first terms in the expansion in order to make the resulting Hamiltonian manageable. Then, as pointed out by Arovas and Auerbach [7], the excellent agreement with the Bethe *ansatz* and numerical results obtained in [2–5] is astonishing, since the constraint guarantees that $\langle a^\dagger a/2S\rangle = \frac{1}{2}$, which hardly justifies the truncation of the aforementioned expansion.

In the present work we focus on this last point. Instead of adding a constraint by hand we will try to improve on conventional SWT by expanding the square root in terms of the shifted operator $a^\dagger a/2S - \alpha$. The shift α will be ultimately determined by the self-consistent condition $\alpha = \langle a^\dagger a/2S\rangle$. For the sake of comparison we apply this procedure to the general quantum antiferromagnet considered in [5]:

$$H = J_1 \sum_{\langle ij\rangle} S_i S_j + J_2 \left(\sum_{\langle ii'\rangle} S_i S_{i'} + \sum_{\langle jj'\rangle} S_j S_{j'} \right) \tag{1}$$

which includes a frustrating next-nearest-neighbour coupling J_2 besides the standard

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nearest-neighbour (isotropic) Heisenberg interaction $J_1 > 0$. The model is defined on a square lattice of N sites, with i, i' belonging to sublattice A and j, j' to sublattice B. We will restrict ourselves to the study of the Néel-ordered ground state of Hamiltonian (1), which is known [8] to exist at least classically for $J_2/J_1 < 0.5$. By taking $J_2 = 0$ we can readily compare our results with those in [3] and [4].

We stress here two important points. First, our procedure leads to a quadratic Hamiltonian and correction (non-harmonic) terms different from those in Takahashi's theory. Secondly, very much like in the constrained theory, the self-consistent condition introduces a gap in the spin-wave excitation spectrum. This allows us to apply the approximation directly to finite lattices in order to compare the results with those obtained from exact diagonalization of small systems (naive application of conventional SWT on finite lattices gives divergent results). As shown below, for $J_2/J_1 \simeq 0$ our results are slightly worse than those in [3–5] but they improve substantially on these for higher levels of frustration, where the constrained theory strongly overestimates the disordering effect.

By means of antiferromagnetic Holstein–Primakoff transformations [6] on sublattices A and B:

$$S_i^+ = (2S)^{1/2}(1 - a_i^\dagger a_i/2S)^{1/2} a_i \qquad S_i^- = (S_i^+)^\dagger \qquad S_i^z = S - a_i^\dagger a_i$$

$$S_j^+ = (2S)^{1/2} b_j^\dagger (1 - b_j^\dagger b_j/2S)^{1/2} \qquad S_j^- = (S_j^+)^\dagger \qquad S_j^z = -S + b_j^\dagger b_j$$

and the further expansion of the square roots to first order in $a_i^\dagger a_i/2S - \alpha$, a general biquadratic Hamiltonian in Bose operators is obtained. Keeping only the harmonic part, Bogoliubov diagnonalization gives

$$H' = \tfrac{1}{2} \sum_k \omega_k (\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k) + \text{constant} \tag{2}$$

where

$$\omega_k = J_1 Sz[(1 - \alpha)/\eta_k](1 - \eta_k^2 \gamma_k^2)^{1/2}$$

and $\gamma_k = \frac{1}{2}(\cos k_x + \cos k_y)$. This dispersion relation differs from the conventional spin-wave dispersion essentially due to the presence of the factor

$$\eta_k = (1 - \alpha)/\{1 + (J_2/J_1)[(1 - \alpha)\Gamma_k - 1]\} \qquad (\Gamma_k = \cos k_x \cos k_y)$$

which introduces a gap for $\alpha > 0$. The actual value of α is determined by the self-consistent equation

$$\alpha = \left\langle \frac{a_i^\dagger a_i}{2S} \right\rangle_0 = \frac{1}{4S} \left(\frac{1}{N} \sum_k \frac{1}{(1 - \eta_k^2 \gamma_k^2)^{1/2}} - 1 \right) \tag{3}$$

where $\langle \hat{A} \rangle_0$ means the expectation value of $\hat{A}$ taken in the ground state of Hamiltonian (2).

Further improvement of the approximation can be achieved by including terms quartic in Bose operators. In this way, we found for the ground-state energy and correlation functions

$$\langle H \rangle_0 = -(zNJ_1/2)(S' + g(\delta))^2 + (zNJ_2/2)(S' + f(\delta'))^2 \tag{4a}$$

$$\langle S_i S_j \rangle_0 = (S' + g(r_i - r_j))^2 \tag{4b}$$

$$\langle S_i S_{i'} \rangle_0 = \langle S_j S_{j'} \rangle = (S' + f(r' - r))^2 - \tfrac{1}{4}\delta_{r,r'} \tag{4c}$$

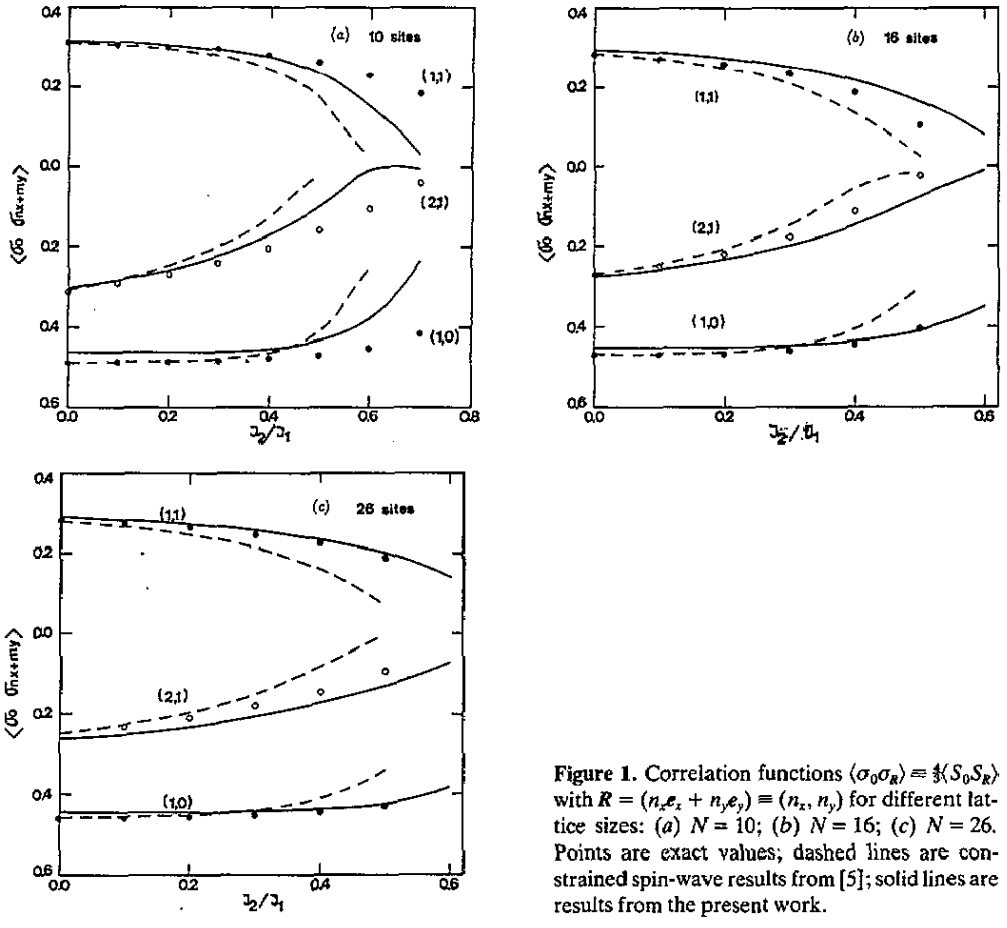

Figure 1. Correlation functions $\langle\sigma_0\sigma_R\rangle \equiv \frac{1}{4}\langle S_0 S_R\rangle$ with $R = (n_x e_x + n_y e_y) \equiv (n_x, n_y)$ for different lattice sizes: (*a*) $N = 10$; (*b*) $N = 16$; (*c*) $N = 26$. Points are exact values; dashed lines are constrained spin-wave results from [5]; solid lines are results from the present work.

where $S' = S(1 - 2\alpha)$ and $\boldsymbol{\delta}, \boldsymbol{\delta}'$ are vectors to nearest and next-nearest neighbours of a given site. We have made the definitions

$$f(\boldsymbol{R}) = \langle a_0^\dagger a_R\rangle_0 + \tfrac{1}{2}\delta_{0,R} = \frac{1}{2N}\sum_k \frac{1}{(1-\eta_k^2\gamma_k^2)^{1/2}}\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}}$$

$$g(\boldsymbol{R}) = \langle a_0 b_R\rangle_0 = \frac{1}{2N}\sum_k \frac{\eta_k\gamma_k}{(1-\eta_k^2\gamma_k^2)^{1/2}}\, e^{i\boldsymbol{k}\cdot\boldsymbol{R}}.$$

From (3) and (4*c*), the proper normalization $\langle S^2\rangle_0 = S(S+1)$ can be easily checked.

Numerical evaluation of (4*b*) and (4*c*) for lattices of different sizes gives the results shown in figure 1. As can be seen, for high degrees of frustration our approach gives better results than those from the constrained SWT [5]. This is particularly so for the largest lattice for which exact numerical results are available ($N = 26$). On the other hand, and contrary to Takahashi's theory which overestimates the disordering effect due to frustration, our approximation tends to underestimate this effect with increasing

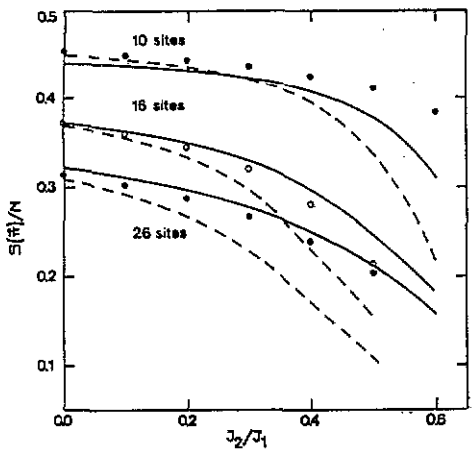

Figure 2. Rotationally averaged structure factor per site for lattice sizes $N = 10, 16, 26$. Points are exact values; dashed lines are constrained spin-wave results from [5]; solid lines are results from the present work.

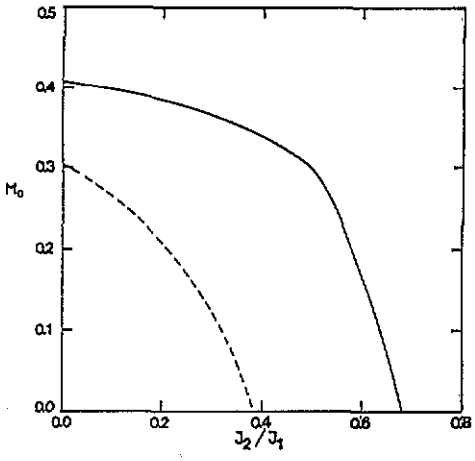

Figure 3. Magnetization per site for the infinite lattice. The dashed line is the conventional spin-wave result from [8]; the solid line is the result from the present work.

lattice size. Both conclusions are even more apparent from the behaviour of the (rotationally averaged) structure factor

$$S(\pi, \pi) = \tfrac{1}{3} \sum_R (-1)^R \langle S_0 S_R \rangle_0$$

which is plotted in figure 2. The predicted values are better than those of [5] and, other than for the smallest lattice ($N = 10$), slightly higher than the exact ones.

It is also interesting to consider the behaviour of the magnetization as a function of J_2/J_1 in the thermodynamic limit. Either from $S(\pi, \pi) = Nm^2 + O(\sqrt{N})$ or the $|r' - r| \to \infty$ limit of (4*b*) and (4*c*) we obtain

$$m = S(1 - 2\alpha) \qquad (N \to \infty). \tag{5}$$

Notice that this is the result one would have obtained from direct calculation of $\langle S^z \rangle$ and further use of the consistency equation (3). Figure 3 shows a plot of m as given by (3)–(5), together with the corresponding result as predicted by the constrained theory [5] (which coincides with the prediction of the conventional SWT [8]). Although our approximation certainly overestimates the stability of the Néel order, numerical results on finite lattices [9] suggest that this order is in fact destroyed for J_2/J_1 around 0.6, which is not too far from the value where m goes to zero in figure 3. In any case, from the discussion of the structure factor behaviour both curves in this figure can be considered upper and lower bounds to the actual magnetization.

In conclusion, a simple modification of standard SWT based on Holstein–Primakoff transformation produces fairly good results for frustrated spin systems. Moreover, for high degrees of frustration it gives results considerably better than those obtained from a similar approximation [2–5] recently considered in the literature.

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