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Towards Spin-Wave Like Approach to the J–J' Heisenberg Antiferromagnet in Terms of Composite Spins

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Conventional spin-wave approach relies on an expansion around a relevant classical (unentangled) ground state or equivalently the ground state in the mean field approximation for the quantum model. However, for systems which may admit valence bond ground states, such as the staggered J–J' Heisenberg antiferromagnet, single site mean field approximation is obviously an incorrect zeroth order approximation. In this paper, we introduce a mean field approximation for clusters consisting of two spins connected by a strong bond in the aforementioned model. We identify the quantum critical point and calculate the ground state magnetization within this cluster mean field approximation in one and two dimensions. Finally, we derive an effective dimer Hamiltonian, in the standard basis operator formalism, which may be a basis for further spin-wave like expansions around the cluster mean field approximation ground state.

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1. Introduction

Low dimensional Heisenberg antiferromagnets (HAFM) play an important role in the field of quantum magnetism due to the plethora of phases and quantum critical points (QCP) they exhibit. In particular, systems with non-uniform couplings such as bilayer or dimerized HAFM offer the possibility of studying quantum phase transitions from antiferromagnetically ordered Néel state (NS) to valence bond (VB) phase, without the complication of additionally introducing frustration. In this paper, we specialize to the dimerized HAFM (so-called J–J' model) with "staggered" distribution of strong bonds (Fig. 1). Recently, it has been suggested in [1] that the NS to VB phase transition in this model may be described as a confinement–deconfinement transition and may belong to different universality class than the Heisenberg O(3) classical universality class in three dimensions. Indeed, the latest quantum Monte Carlo (QMC) simulations [2] seem to confirm the latter claim. It seems therefore important to study the aforementioned model in detail.

The staggered J–J' model was examined by series expansion method [3], renormalized spin-wave (RSW) approach [4], exact diagonalization and the coupled cluster method [5], and QMC simulations [6, 2]. Most of these metods predict a single, continuous quantum phase transition between NS and VB phases for J'/J ratio close to 2.5, with only RSW grossly overestimating this ratio as 5.0. The latter result is suprising, since spin-wave expansion is known as one of the most powerful methods in the theory of low dimensional magnetic systems. The apparent failure of RSW seems intuitively to be connected with the fact that unlike in Néel ordered states, single site mean field approximation (MFA) clearly is an incorrect zeroth order approximation for states with VB order, as in the staggered J–J' HAFM. Conventional spin-wave approach centrally relies on an expansion around a classical ground state or equivalently the ground state in the MFA for the quantum model — indeed in the frustrating regime $J' < 0$, when the ground state may be approximated by a classical helical state the RSW works quite

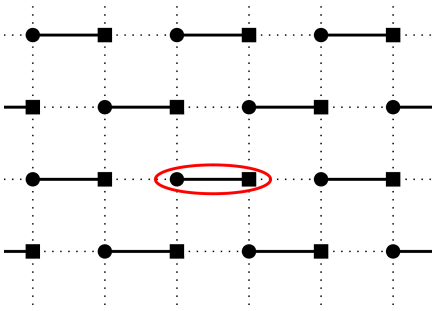

Fig. 1. Distribution of bonds for staggered J–J' HAFM model. Thick lines denote stronger J' bonds, dotted lines weaker J bonds. Square lattice is divided on sublattice A (circles) and B (squares). One of the dimers is marked by an elipse.

well [4]. Therefore in this paper, we introduce an MFA for dimers, in the hope of developing a spin-wave like expansion for dimers viewed as a composite $\frac{3}{2}$ spins. The J–J' HAFM Hamiltonian on the square lattice reads

$$H = J' \sum_{\langle i,j\rangle'} \boldsymbol{S}_i \boldsymbol{S}_j + J \sum_{\langle i,j\rangle} \boldsymbol{S}_i \boldsymbol{S}_j = H_{\rm dim} + H_{\rm int}, \quad (1)$$

where both sums run over pairs of nearest neighbors. The first sum over $\langle i,j\rangle'$ includes strong, intra-dimer, bonds with coupling constant ($J' > J > 0$), while the sum over $\langle i,j\rangle$ includes inter-dimer bonds with coupling constant J. Let us note that the staggered distribution of strong bonds (Fig. 1) consists of pairs of sites belonging to sublattices A and B taken in the same order. Therefore, if we introduce the "dimer site" number l, we can unambiguously relabel all the original lattice sites by their dimer number supplemented by the sublattice label (A or B), so that the $H_{\rm dim}$ and $H_{\rm int}$ can be written as

$$H_{\rm dim} = J' \sum_{l} \left[\frac{1}{2}(S^+_{A,l} S^-_{B,l} + S^-_{A,l} S^+_{B,l}) + S^z_{A,l} S^z_{B,l} \right],$$
$$H_{\rm int} = J \sum_{l,\delta} \left[\frac{1}{2}(S^+_{A,l} S^-_{B,l+\delta} + S^-_{A,l} S^+_{B,l+\delta}) + S^z_{A,l} S^z_{B,l+\delta} \right], \quad (2)$$

where δ is one of the 3 vectors emerging to the left of a given dimer connecting it with its nearest neighbors (see Fig. 2).

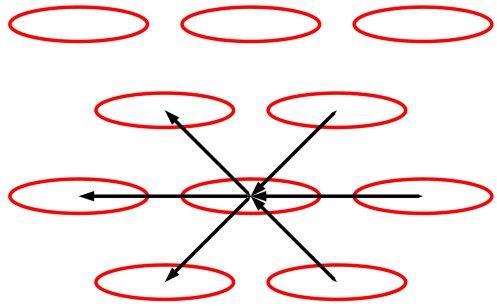

Fig. 2. Effective lattice for dimers is triangular. Bonds are directed. Interaction of spin A from one dimer with spin B from another dimer is denoted by an arrow (from A to B). The index δ in the text, refers to the set of bonds pointing out of the dimer.

2. Mean field approximation for dimers

In this section, we consider an approximation within which interactions on strong bonds are treated exactly, while other interactions are considered in a standard mean field manner. This leads to the following Hamiltonian (up to a constant term) of noninteracting dimers in an effective field:

$$H_{\rm MF} = \sum_{l} \left\{ J' \left[\frac{1}{2}(S^+_{A,l} S^-_{B,l} + S^-_{A,l} S^+_{B,l}) + S^z_{A,l} S^z_{B,l} \right] + J(z-1)m(S^z_{A,l} - S^z_{B,l}) \right\}, \quad (3)$$

where $m = \langle S^z_B \rangle = -\langle S^z_A \rangle$ and z is the coordination number of the original lattice (let us note that the term $(z-1)m$ multiplies each spin in a dimer, hence the dimer treated as an entity has $2(z-1)$ nearest neighbors in the effective lattice in accordance with Fig. 2). The eigenstates of a single dimer take the form

$$|1\rangle = \sin\phi|\uparrow\downarrow\rangle - \cos\phi|\downarrow\uparrow\rangle, \quad |3\rangle = |\uparrow\uparrow\rangle,$$
$$|2\rangle = \cos\phi|\uparrow\downarrow\rangle + \sin\phi|\downarrow\uparrow\rangle, \quad |4\rangle = |\downarrow\downarrow\rangle, \quad (4)$$

where $\sin 2\phi = \frac{J'}{J(z-1)}$ for $J' < J(z-1)$ and 1 otherwise. Here, $|1\rangle$ is the dimer ground state with energy $E_0 = -\frac{J'}{4} - \frac{J(z-1)}{2}$ for $J' < J(z-1)$ and $-\frac{3J'}{4}$ otherwise. We note that this ground state form coincides with the trial variational function considered in [5]. In the notation of Eq. (4), the sublattice magnetization $m = \frac{1}{2}\cos 2\phi$, which leads to

$$m = \frac{1}{2}\sqrt{1 - \left[\frac{J'}{J(z-1)}\right]^2}, \quad (5)$$

for $J' < J(z-1)$ and 0 otherwise. A quantum phase transition from Néel to VB phases occurs for $J'/J = z-1$, which for the square lattice is 3.0 — a quite promising value considering the simplicity of the approximation. The above treatment can also be applied to the one-dimensional dimerized J–J' HAFM system yielding a critical value $J'/J = 1$, which in this case happens to be exact. Therefore, it seems that the described MFA for dimers is a good zeroth order approximation, on top of which a low energy effective theory, analogous to spin-wave expansion, can be constructed by treating the dimers as composite four-level systems (abstract spin-$\frac{3}{2}$ sites). Unfortunately, interactions between dimers, described in terms of the standard spin-$\frac{3}{2}$ operators are rather cumbersome. A more fruitful avenue in this regard is to resort to the standard basis operator (SBO) formalism [7].

3. The Hamiltonian in SBO formalism

The standard basis operators form the simplest matrix basis for (sub)systems with a finite number of states. With respect to a given chosen basis of states (here denoted by the first letters of the Greek alphabet) corresponding to a subsystem at a given site l, the standard basis operators are $L^l_{\alpha\beta} = |\alpha^l\rangle\langle\beta^l|$, i.e.

$$L^l_{\alpha\beta}|\gamma^l\rangle = \delta_{\beta\gamma}|\alpha^l\rangle \quad \text{and} \quad (L^l_{\alpha\beta})^\dagger = L^l_{\beta\alpha}. \quad (6)$$

Choosing each site to now correspond to a dimer, we can write the original spin-$\frac{1}{2}$ operators in the basis of dimer states (4) (where ϕ is to be determined once again):

$$S^+_{A,l} = \sin\phi(L^l_{32} + L^l_{14}) + \cos\phi(L^l_{24} - L^l_{31}),$$
$$S^-_{A,l} = (S^+_{A,l})^\dagger,$$
$$S^+_{B,l} = \cos\phi(L^l_{32} - L^l_{14}) + \sin\phi(L^l_{24} + L^l_{31}),$$
$$S^-_{B,l} = (S^+_{B,l})^\dagger,$$
$$2S^z_{A,l} = \sin 2\phi(L^l_{12} + L^l_{21}) - \cos 2\phi(L^l_{11} - L^l_{22})$$

$$+L^l_{33} - L^l_{44},$$

$$2S^z_{B,l} = -\sin 2\phi(L^l_{12} + L^l_{21}) + \cos 2\phi(L^l_{11} - L^l_{22})$$

$$+L^l_{33} - L^l_{44}. \quad (7)$$

Using (7) we can now recast original Hamiltonian (1) into the form

$$H = -\sum_{l,\alpha\alpha'} h_{\alpha\alpha'} L^l_{\alpha\alpha'} - \sum_{l,\delta} \sum_{\alpha\alpha',\beta\beta'} T_{\alpha\alpha',\beta\beta'}(l, l+\delta) L^l_{\alpha\alpha'} L^{l+\delta}_{\beta\beta'}, \quad (8)$$

where the non-zero elements of matrix $[h]$ are

$$h_{11} = J'\left(\frac{1}{2} + \sin 2\phi\right)/2,\ h_{22} = J'\left(\frac{1}{2} - \sin 2\phi\right)/2,$$

$$h_{33} = h_{44} = -J'/4, \quad h_{12} = h_{21} = J'/2\cos 2\phi, \quad (9)$$

and the tensor $[T]$ consists of 256 elements of which the non-zero read

$$T_{32,23} = T_{42,24} = T_{24,13} = T_{12,33} = T_{44,12} = -\frac{J}{4}\sin 2\phi, \quad (10a)$$

$$T_{31,13} = T_{41,14} = T_{13,24} = T_{23,14} = T_{12,44} = T_{33,12} = \frac{J}{4}\sin 2\phi, \quad (10b)$$

$$T_{32,42} = T_{32,13} = T_{41,24} = T_{41,31} = -\frac{J}{2}\sin^2\phi, \quad (10c)$$

$$T_{42,32} = -T_{13,32} = -T_{24,41} = T_{31,41} = -\frac{J}{2}\cos^2\phi, \quad (10d)$$

$$T_{11,11} = T_{22,22} = -T_{22,11} = -T_{11,22} = \frac{J}{4}\cos^2 2\phi, \quad (10e)$$

$$T_{12,21} = T_{21,12} = T_{12,12} = T_{21,21} = \frac{J}{4}\sin^2 2\phi, \quad (10f)$$

$$T_{33,33} = T_{44,44} = -T_{33,44} = -T_{44,33} = -\frac{J}{4}, \quad (10g)$$

$$-T_{33,11} = T_{11,33} = -T_{44,22} = T_{22,44} = T_{33,22} = -T_{22,33} = T_{44,11} = -T_{11,44} = \frac{J}{4}\cos 2\phi, \quad (10h)$$

$$T_{11,12} = T_{12,11} = -T_{22,12} = -T_{12,22} = -\frac{J}{8}\sin 4\phi, \quad (10i)$$

and $T_{ij,kl} = T_{ji,lk}$. The derivation of the Hamiltonian (8) is the final point of this paper and it forms the basis for further work. Let us notice that the Hamiltonian (8) has a simple bilinear form (typical of the SBO), which should therefore be suitable for further calculations, despite the complicated interactions in the dimer basis. Importantly, decoupling the terms $L^l_{\alpha\alpha'} L^{l+\delta}_{\beta\beta'}$ in (8) in a mean field manner, and setting $\langle L_{11}\rangle = 1$ and all other averages $\langle L_{\alpha\alpha'}\rangle = 0$ leads to the earlier results for the dimer MFA derived in the previous section. Thus, the Hamiltonian (8) is well suited to be treated using the SBO formalism Green function equation of motion method [8], wherein the effects of inter-dimer correlations can be accounted for, allowing the calculation of long-range spin-wave like excitations in this system.

4. Summary and further work

In this paper, we introduced a mean field approximation for clusters consisting of two spins connected by a strong bond in the staggered J–J' Heisenberg antiferromagnet, and showed that this is a good zeroth order approximation for this system. Based on this, we derived an effective dimer Hamiltonian, in the SBO formalism, which to our knowledge has not been hitherto considered in this context. The standard mean field approximation for the latter Hamiltonian results in the introduced cluster mean field approximation. Therefore, the obtained Hamiltonian in the SBO formalism may be a good basis for further spin-wave like expansions around the cluster MFA ground state.

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