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SYSTEMATIC INCLUSION OF MULTI-SPIN CORRELATIONS IN THE SPIN-HALF TRIANGULAR ANTIFERROMAGNET

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ABSTRACT

Multi-spin correlations are crucial in determining the novel magnetic orderings present in spin-lattice models with strong quantum spin fluctuations; but they are difficult to deal with. By applying the coupled cluster method to the spin-half triangular antiferromagnet, we illustrate how a systematic inclusion of multi-spin correlations can be made.

Multi-spin correlations and their competing effects undoubtedly play a crucial role in determining the magnetic phase diagram of a system like solid ^{3}He, where multi-spin exchanges are expected to be important.[1] However, even for simple model systems such as two-dimensional spin-$\frac{1}{2}$ anisotropic antiferromagnets with only nearest-neighbour interactions, they are also of particular significance when quantum spin fluctuations are strong enough to greatly reduce or totally destroy the corresponding classical ordering. In this article we wish to illustrate how the multi-spin correlations can be systematically taken into account within the framework of the coupled cluster method[2] (CCM) by examining specifically the spin-$\frac{1}{2}$ triangular antiferromagnet[3] within a particular type of CCM approximation scheme. The method described below, however, will not only be easy to be implemented numerically but will also be of general utility in dealing with lattice Hamiltonian problems.

The Hamiltonian under consideration can be written as:

$$H = \sum_{k\rho} \left\{ -2s_k^z s_m^z - 2\lambda(s_k^x s_m^x - 2s_k^y s_m^y) + 2\sqrt{3}\lambda(s_k^z s_m^x - s_k^x s_m^z) \right\} , \qquad (1)$$

where $\{s^x, s^y, s^z\}$ are the spin-$\frac{1}{2}$ operators defined with respect to local quantization axes, which are chosen to orient along the spin direction of the classical ground state. Here the summation over k runs over all triangular-lattice sites, while the summation over ρ is over the three nearest-neighbour vectors that point from A to B, B to C, or C to A for a given three-sublattice partition of the triangular lattice with the three sublattices being denoted by A, B, and C respectively. We also henceforth follow a specific convention: $m \equiv k + \rho$ throughout this paper to ease the notational burden. It is easy to show that H describes the conventional Heisenberg antiferromagnet when the anisotropy parameter becomes unity ($\lambda = 1$).

The CCM ansatz for the ground ket state $|\Psi\rangle$ is given by: $|\Psi\rangle = e^S|\Phi\rangle$ where the reference state $|\Phi\rangle$ for the present model is chosen to be the fully aligned ferromagnetic

configuration in the local spin coordinates, i.e., $s_k^z|\Phi\rangle = -\frac{1}{2}|\Phi\rangle$ for any arbitrary site k. Here the spin correlation operator S is decomposed wholly in terms of spin-raising operators, $s_k^+ \equiv s_k^x + is_k^y$,

$$S = [i_1]s_{i_1}^+ + [i_1 i_2]s_{i_1}^+ s_{i_2}^+ + \cdots , \tag{2}$$

where $[i_1]$, $[i_1 i_2]$ and so on stand for the corresponding (symmetric) spin-correlation coefficients specified by the sets of site indices $\{i_1\}$, $\{i_1, i_2\}$ and so on. Implicit summations over double indices are also assumed. Furthermore, the spin-correlation coefficients in Eq. (2) are to be determined by a set of CCM nonlinear eqations:

$$0 = \langle\Phi|s_{j_1}^- s_{j_2}^- \cdots s_{j_M}^- \mathrm{e}^{-S} H \mathrm{e}^{S}|\Phi\rangle , \tag{3}$$

where $s_{j_1}^- s_{j_2}^- \cdots s_{j_M}^-$ is the Hermitian conjugate of the corresponding multi-spin correlation string $s_{j_1}^+ s_{j_2}^+ \cdots s_{j_M}^+$ (and see Ref. [2] for details). It should be noted that the multi-spin correlations that are identical by lattice symmetries, translational and rotational alike, are counted as one single distinct correlation. The implementation of the CCM consists of enumerating the distinct multi-spin correlations retained in a desired approximation and generating the corresponding set of CCM equations. It is on the latter that we will focus in this article. Equation (3) reveals that there are essentially two computational aspects involved in obtaining all possible nonzero contributions to its right-hand side. The first is to calculate the similarity-transformed Hamiltonian which then acts on the reference state, and the second is to select terms of the similarity-transformed Hamiltonian that match exactly the string of spin-lowering operators represented by the set of site indices $\{j_1, j_2, \cdots j_M\}$. The first aspect is intrinsically related to the noncommutative nature of quantum spin operators, and the second to the geometric considerations of the triangular lattice on which the Hamiltonian is defined. We address these two aspects in more detail below.

The similarity-transformed Hamiltonian acting on $|\Phi\rangle$, $\hat{H}|\Phi\rangle \equiv \mathrm{e}^{-S} H \mathrm{e}^{S}|\Phi\rangle$, can be obtained straightforwardly; and all its terms are further classified into three categories, i.e., $\hat{H}|\Phi\rangle = (\hat{H}_1 + \hat{H}_2 + \hat{H}_3)|\Phi\rangle$, as indicated below:

$$\hat{H}_1 = \sum_{k\rho}\left\{-\frac{1}{2} - \frac{\sqrt{3}\lambda}{2}(F_m - F_k) - \frac{3\lambda}{2}(H_{km} + F_k F_m)\right\} \tag{4}$$

$$\begin{aligned}\hat{H}_2 = {} & \sum_{k\rho}\left\{[F_m - \frac{\sqrt{3}\lambda}{2}(1 - F_m^2) + \frac{\lambda}{2}F_k]s_m^+ + [F_k + \frac{\sqrt{3}\lambda}{2}(1 - F_k^2) + \frac{\lambda}{2}F_m]s_k^+\right\} \\ & + \sum_{k\rho}\lambda\left\{\sqrt{3}(H_{km} + F_k F_m)(s_k^+ - s_m^+) + \frac{3}{2}(H_{km} + 2F_k F_m)(F_m s_m^+ + F_k s_k^+)\right\}\end{aligned} \tag{5}$$

$$\begin{aligned}\hat{H}_3 = {} & \sum_{k\rho}\left\{-2(H_{km} + F_k F_m) - \frac{3\lambda}{2} + \sqrt{3}\lambda(F_k - F_m)(1 + 2H_{km} + F_k F_m)\right\} s_k^+ s_m^+ \\ & + \sum_{k\rho}\left\{-\frac{\lambda}{2}(F_m^2 + F_k^2) - 3\lambda H_{km}^2 - 6\lambda H_{km} F_k F_m - \frac{3\lambda}{2}F_k^2 F_m^2\right\} s_k^+ s_m^+ ,\end{aligned} \tag{6}$$

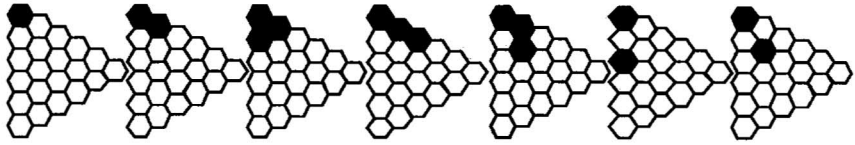

Figure 1: All 7 independent spin correlations retained at the level of LSUB3, where the shaded hexagons mark the relative positions of the sites of the triangular lattice on which the spins are flipped with respect to the reference state.

where $F_k \equiv \sum_l l[ki_1 \cdots i_{l-1}] s^+_{i_1} \cdots s^+_{i_{l-1}}$, with a similar definition for F_m, and $H_{km} \equiv \sum_l l(l-1)[kmi_1 \cdots i_{l-2}] s^+_{i_1} \cdots s^+_{i_{l-2}}$.

The reason for such a classification becomes clear when we consider the second aspect of generating the CCM equations. Thus, for example, in $\hat{H}_3$ all of the site indices of its terms, including both k and m, are completely fixed up to permutations by the set of indices $\{j_1, j_2, \cdots j_M\}$ under consideration in evaluating Eq. (3). By contrast, neither index k nor m need belong to the set $\{j_1, j_2, \cdots j_M\}$ in (the last term of) $\hat{H}_1$, and in $\hat{H}_2$ only one need do so. The terms $\hat{H}_2$ and $\hat{H}_1$ hence require more computational effort for their evaluation. Nevertheless, for a class of approximation schemes usually used in CCM applications, e.g., the systematic LSUBm scheme described below, both k and m must lie within a finite set of indices for which $\{j_1, j_2, \cdots j_M\}$ is a subset. The search for all k and m that give rise to nonzero contributions from each of the terms in $\hat{H}_2$ and $\hat{H}_1$ is then readily implemented, since all of the terms and their explicit structure are completely given in Eqs. (4) and (5).

In the so-called LSUBm scheme, all multi-spin correlations over all possible distinct locales on the triangular lattice defined by at most m contiguous lattice sites are retained. We find that the corresponding number of distinct multi-spin correlations for the sequence of LSUBm with $m = 2, 3, 4$, and 5 is $2, 7, 21$, and 89 respectively. For example, all 7 distinct correlations for LSUB3 are shown in Fig. 1.

In Fig. 2 we show the ground-state energy per spin, $e_g(\lambda) \equiv E_g(\lambda)/N$, as a function of the anisotropy parameter λ for LSUB2, LSUB3, and SUB2 (all two-spin correlations are retained in SUB2). In particular, SUB2 yields $e_g(\lambda = 1) = -2.015$ for the isotropic Heisenberg point[4] (which should be compared with the corresponding classical value of -1.5, the value -2.028 obtained by variational calculations where the nearest-neighbour two-spin correlations are retained[5], and the value -2.21 ± 0.01 extrapolated from the series expansion[3]), while LSUB3 is found to yield an improved value of -2.078 (which should be compared with the value -2.112 obtained by a variational wave function where only nearest-neighbour two-spin and three-spin correlations are included[6]). Clearly the CCM results compare well with those from variational methods when the levels of multi-spin correlations retained are comparable. Moreover, the CCM calculations can be easily extended to higher orders. The

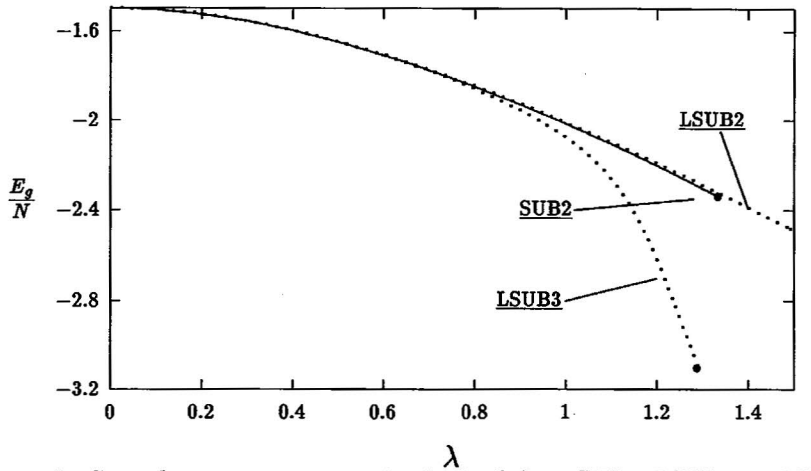

Figure 2: Ground-state energy per spin obtained from SUB2, LSUB2, and LSUB3 approximations. Note that the ground-state energy as a function of the anisotropy parameter λ terminates for both SUB2 and LSUB3 approximations.

CCM equations of higher-order truncation schemes such as LSUB4 and LSUB5 have been generated, and the results of more detailed studies, including the nature[7] of the ground-state energy criticalities observed here already in SUB2 and LSUB3 approximations, will be reported elsewhere.

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