Spin-wave expansion of the ground-state energy of the square-lattice Heisenberg antiferromagnet

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A spin-wave expansion is used to compute the ground-state energy of the square-lattice Heisenberg antiferromagnet to order $1/s$. It is found that the ground-state energy per bond, $\mathcal{E}_0$, is given by $\mathcal{E}_0=-s^2-0.157\,947s-0.006\,237s^0+0.000\,107s^{-1}+O(s^{-2})$. For $s=\frac{1}{2}$, this expression gives the value $\mathcal{E}_0=-0.3350$, which is in good agreement with the more precise Green's-function Monte Carlo and series-expansion estimates of the ground-state energy.

The Hamiltonian for square-lattice Heisenberg antiferromagnet,

$$H=\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\ , \tag{1}$$

where the sum extends over distinct pairs of nearest neighbors, has attracted much attention in recent years among physicists.[1-13] The square-lattice $s=\frac{1}{2}$ Heisenberg Hamiltonian (1) is assumed to describe the antiferromagnetic, undoped insulator La_2CuO_4 or the oxygen-deficient $YBa_2Cu_3O_6$ or other undoped copper oxide materials (for a review see Ref. 1). It has been suggested that an investigation of magnetism in these materials may lead to a better understanding of the nature of high-temperature superconductivity.[1,2,14]

Despite its simple form, the Heisenberg Hamiltonian (1) appears to be a great theoretical challenge. The exact solution for the ground state and excitations is known only for the $s=\frac{1}{2}$ chain.[15] Unfortunately, Bethe's[15] method cannot be generalized to the investigation of higher-dimensional systems. A number of approximate and numerical methods has lately been developed and applied to the theoretical investigation of the spectral characteristics of the two-dimensional model (1).[1,3-13] Experiments with La_2CuO_4 and other quasi-two-dimensional systems have also been carried out.[14] Important results have been obtained, but the problem of the ground state of the square-lattice Heisenberg antiferromagnet has not yet received a definitive solution.[1]

At present, there is considerable numerical evidence showing that the ground state of the square-lattice model (1) has a finite sublattice magnetization m, whose exact value is still under discussion. Published theoretical estimates of m for $s=\frac{1}{2}$ vary from $m=0.24$ to $m=0.43$ (see Ref. 1 and the references therein). The experimental situation is also unsettled, mainly because the staggered magnetization of La_2CuO_4 strongly correlates with the oxygen content of the sample.[14] Clearly discernible, although smaller differences are found in estimates[1] of the ground-state energy E_0.

One way to obtain precise estimates of E_0 and m is connected with calculation of the corrections within the framework of spin-wave theory. It is well known that corrections to the classical Néel state in this theory may be expanded as a power series in $1/s$. It turns out[1,16-18] that although asymptotic, these spin-wave expansions may be quite useful for a general understanding of square-lattice antiferromagnet characteristics even for $s=\frac{1}{2}$. This has been most convincingly demonstrated recently in Refs. 3, 9-11. Castilla and Chakravarty,[3] using the Dyson-Maleev (DM) formalism, calculated the $O(1/s^2)$ term in the spin-wave (SW) expansion of m and concluded that

$$m=s-0.196\,60s^0+0s^{-1}-0.000\,68s^{-2}+O(s^{-3})\ . \tag{2}$$

The first two terms in (2) are known from the linear spin-wave theory of Anderson[16] and Kubo,[17] which also gives the first two terms in the expansion of E_0. The third term in (2), as well as the corresponding $O(1)$ term in the expansion of E_0, are calculated in Ref. 18 by accounting for the magnon-magnon interaction to the lowest order. The power series (2) of m generates asymptotically small terms and therefore the theory is self-consistent up to this order.[3] The values of m, obtained from (2) for $s=\frac{1}{2}$ and $s=1$, are in agreement with the results of recent numerical calculations.[3,7,8]

Similar higher-order SW calculations of the self-energy and spin-wave velocity in the DM formalism have been performed by Canali and co-workers.[9,11] Using the Holstein-Primakoff (HP) transformation, Igarashi and Watabe[10] have calculated corrections to the self-energy and magnetization. Although some discrepancy[19] between published results[3,10,11] exists, these investigations demonstrate how useful spin-wave expansions can be.

In the present work the spin-wave expansion, to $O(1/s)$, of the ground-state energy of the square-lattice Heisenberg system (1) has been determined. The result obtained shows that the expansion of E_0 up to this order generates small corrections and gives very good estimates of the energy.

We shall use the DM formalism which is the most tractable in terms of number of well-behaved spin-wave–spin-wave interaction vertices.[3,4,9,11,20] It is known[3,9] that all infrared singularities in the DM scheme cancel out order by order. This property is not shared by the HP formalism. The introduction of bosons in model (1) through the DM transformation and the diagonalization of the corresponding quadratic form have been con-

sidered many times in the literature (see, for example, Refs. 3, 4, and 20). Here we shall give only the final result for the square-lattice Hamiltonian (1), expressed with the u-v bosons $\alpha_{\mathbf{k}}$, $\beta_{\mathbf{k}}$ in the form presented in[20]:

$$H_{\mathrm{DM}}=-2s^2N-4s\sum_{\mathbf{k}}(1-\varepsilon_{\mathbf{k}})+H^{(2)}+H^{(4)}\ , \tag{3}$$

where N is the number of sites, $-2s^2N$ is the energy of the Néel state; $-4s\sum_{\mathbf{k}}(1-\varepsilon_{\mathbf{k}})$ is the energy of zero-point fluctuations; $E_{\mathbf{k}}=4s\varepsilon_{\mathbf{k}}$ is the energy of the spin wave; $\varepsilon_{\mathbf{k}}=[1-\gamma^2(k)]^{1/2}$ is the corresponding dimensionless energy; $\gamma(\mathbf{k})=(\cos k_x+\cos k_y)/2$;

$$H_2=\sum_{\mathbf{k}}E_{\mathbf{k}}(\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}+\beta_{\mathbf{k}}^{\dagger}\beta_{\mathbf{k}}) \tag{4}$$

is the Hamiltonian of the noninteracting spin waves; and $H^{(4)}$ is the magnon-magnon interaction operator. The expression for $H^{(4)}$ obtained in Ref. 20 (see also Refs. 3,4, and 9) shall not be repeated here. One should note that $H^{(4)}\sim O(1)$, whereas $H^{(2)}$ [easily seen from (4)] is proportional to s. Therefore, for the characteristics of the Hamiltonian $H^{(2)}+H^{(4)}$ formal expansions in the power of $1/s$ can be constructed, with $H^{(4)}$ treated as a perturbation.

The first-order correction to the ground-state energy

$$\Delta E_0^{(1)}=\langle H^{(4)}\rangle$$

is calculated in Refs. 12, 18, and 21. From this correction and the constants in (3) the first three terms in the spin-wave expansion of E_0,

$$\mathcal{E}_0\equiv E_0/2N=-a_0s^2-a_1s-a_2s^0+a_3s^{-1}+\cdots \tag{5}$$

are obtained:[12]

$$a_0=1,\quad a_1=(2/N)\sum_{\mathbf{k}}(1-\varepsilon_{\mathbf{k}})=0.157\,947\ ,$$
$$a_2=(a_1/2)^2=0.006\,237\ . \tag{6}$$

The quantity $\mathcal{E}_0$ represents the energy per bond. The energy per site in the case considered is $2\,\mathcal{E}_0$.

Our aim here is to calculate the correction $\Delta E_0^{(2)}$, from which the coefficient a_3 in the expansion (5) can be determined. It is well known[22] that the expression for the second-order correction to the ground-state energy in the case of Hermitian operator of interaction

$$\Delta E_0^{(2)}=-\sum_{\langle\rho\rangle}\frac{\langle 0|H^{(4)}|\rho\rangle\langle\rho|H^{(4)}|0\rangle}{E_\rho} \tag{7}$$

may be applied as well in the case of non-Hermitian operator of the interaction considered here, namely, $H^{(4)}$. In (7), $|0\rangle$ and $|\rho\rangle$ are the ground and excited states of $H^{(2)}$, respectively ($E_0^{(0)}=0$).

Analyzing the $H^{(4)}$ structure, one sees that only definite states of $H^{(2)}$, namely, the states

$$|\rho\rangle=\alpha_{\mathbf{q}_1}^{\dagger}\alpha_{\mathbf{q}_2}^{\dagger}\beta_{\mathbf{q}_3}^{\dagger}\beta_{\mathbf{q}_4}^{\dagger}|0\rangle\ ,$$

where $\mathbf{q}_1+\mathbf{q}_2-\mathbf{q}_3-\mathbf{q}_4=\mathbf{0}$ or $\mathbf{K}$, $\mathbf{K}$ being a reciprocal-lattice vector, contribute to the sum over ρ in (7). After that, the matrix element $\langle O|H^{(4)}|\rho\rangle$ is easily obtained:

$$\langle 0|H^{(4)}|\rho\rangle=(-8/N)V^{(8)}_{(3412)}\Delta(1+2-3-4)\ , \tag{8}$$

where $\Delta(1+2-3-4)$ is the Kronecker delta function and the vertex $V^{(8)}$ is given by the expression[9]

$$V^{(8)}_{(3412)}=v_1v_2[\gamma(4-1-2)v_3u_4+\gamma(3-1-2)v_4u_3]+u_1u_2[\gamma(4)v_3u_4+\gamma(3)v_4u_3]$$
$$-[\gamma(2-4)v_3u_1v_2u_4+\gamma(1-4)v_3u_2v_1u_4+\gamma(2-3)v_4u_1v_2u_3+\gamma(1-3)v_4u_2v_1u_3]\ . \tag{9a}$$

Here $1\equiv\mathbf{q}_1$, $u_{\mathbf{q}}=[(1+\varepsilon_{\mathbf{q}})/2\varepsilon_{\mathbf{q}}]^{1/2}$, and $v_{\mathbf{q}}=[(1-\varepsilon_{\mathbf{q}})/2\varepsilon_{\mathbf{q}}]^{1/2}$. For the matrix element $\langle\rho|H^{(4)}|0\rangle$ we have $\langle\rho|H^{(4)}|0\rangle=(-8/N)V^{(7)}_{(1234)}\Delta(1+2-3-4)$, where[9]

$$V^{(7)}_{(1234)}=v_3v_4[\gamma(1)v_1u_2+\gamma(2)v_2u_1]+u_3u_4[\gamma(2-3-4)v_2u_1+\gamma(1-3-4)v_1u_2]$$
$$-[\gamma(2-4)v_3u_1v_2u_4+\gamma(1-4)v_3u_2v_1u_4+\gamma(2-3)v_4u_1v_2u_3+\gamma(1-3)v_4u_2v_1u_3]\ , \tag{9b}$$

Further transformations of (7) lead to the following result:

$$\Delta E_0^{(2)}/2N=(1/s)a_3\ ,\quad \sum_{(\rho)}\cdots=(1/4)\sum_{(1234)}\cdots\ ,$$

and

$$a_3=-(2/N^3)\sum_{(1234)}\Delta(1+2-3-4)\frac{V^{(7)}_{(1234)}V^{(8)}_{(3412)}}{\varepsilon_1+\varepsilon_2+\varepsilon_3+\varepsilon_4}\ . \tag{10}$$

The long-wavelength singularities of the integrand in (10) can be most easily studied by using the parametrization of the DM vertices (9) proposed in Refs. 3 and 4. Our analysis of the singularities of (10) resembles the analysis of the singularities of the $O(1/s^2)$ correction to the staggered magnetization made in Ref. 3. After some algebraic manipulations, it can be proved that the integrand in (10) has an integrable singularity at the point $\mathbf{q}_1=\mathbf{q}_2=\mathbf{q}_3=\mathbf{q}_4=\mathbf{0}$ and discontinuities at points $\mathbf{q}_1=\mathbf{0}$, $\mathbf{q}_2=\mathbf{0}$, $\mathbf{q}_3=\mathbf{0}$, and $\mathbf{q}_4=\mathbf{0}$. As a consequence we have $|\Delta E_0^{(2)}|<\infty$, i.e., the calculation of $\Delta E_0^{(2)}$ in the DM formalism does not lead to a divergence.

To calculate numerically the integral in (10), the integrand at the singularity points was determined by making a Taylor expansion, performed at the neighboring nonsingular ponts. The calculations were carried out on a sequence of condensing grids. The grid step was chosen in such a way that the precision of the coefficient a_3, quoted below in (11) is guaranteed.

As has been shown in Refs. 9 and 11, a correct treatment of umklapp processes is essential for the calculation of the spin-wave velocity. We checked here the impor-

tance of umklapp processes by evaluating the integral (10) in two different ways. Assuming that the umklapp process is not essential for a_3, we replaced in integrand 3 by $1+3$ and 4 by $2-3$ and we integrated over $\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3$ in the Brillouin zone (BZ). This way $a_3=-0.000\,263$ was obtained. After that we accounted correctly for umklapp processes, taking $\mathbf{q}_4=\mathbf{q}_1+\mathbf{q}_2-\mathbf{q}_3$ if $\mathbf{q}_1+\mathbf{q}_2-\mathbf{q}_3$ is within BZ or $\mathbf{q}_4=\mathbf{q}_1+\mathbf{q}_2-\mathbf{q}_3-\mathbf{K}$ if $\mathbf{q}_1+\mathbf{q}_2-\mathbf{q}_3$ is outside BZ. In this case a very different value for a_3, namely, $a_3=0.000\,107$, was obtained. This difference demonstrates the importance of umklapp processes in the calculation of higher-order corrections to the ground-state energy.

With a_3 calculated in this way and with use of expression (6), we obtain the following expansion for the ground-state energy per bond of the square-lattice Heisenberg antiferromagnet:

$$\mathcal{E}_0=-s^2-0.157\,947s-0.006\,237s^0 +0.000\,107s^{-1}+O(s^{-2})\ . \tag{11}$$

The absolute values of the coefficients of expansion (11) decrease and the corrections due to the last two terms are small. The first three terms in (11) for $s=\frac{1}{2}$ give[1,18,21,22] $\mathcal{E}_0=-0.3352$. The inclusion of the $O(1/s)$ term in the expansion of $\mathcal{E}_0$ rises this energy to $\mathcal{E}_0=-0.3350$. The latter value is in good agreement with the more precise estimate $\mathcal{E}_0=-0.334\,65$, obtained by the series expansion of Zheng, Oitmaa, and Hamer[12] and by the Green's-function Monte Carlo method of Runge[13] (the other numerical estimates of $\mathcal{E}_0$ are reviewed in Refs. 1 and 12). For $s=1$, the result from (11) is $\mathcal{E}_0=-1.1641$, which is in agreement with the estimate $\mathcal{E}_0=-1.1635\pm0.0005$, calculated by use of series expansion around the Ising limit.[8]

Recently, using both the Dyson-Maleev and Holstein-Primakoff formalisms, Hamer, Zheng, and Arndt[23] and Zheng and Hamer[24] have considered, in particular, the $O(1/s)$ term in the spin-wave expansion of of E_0 and they have evaluated this term by methods different than ours. Their results for a_3, namely $a_3=0.000\,108(3)$ Ref. 23 and $a_3=0.0001071(1)$ Ref. 24 are in full agreement with Eq. (11) of the present work.

These results show that spin-wave expansion to $O(1/s)$ (11) is a useful expansion for calculation of the ground-state energy of the square-lattice Heisenberg antiferromagnet.

In the present consideration we have ignored effects caused by the introduction of the infinite-dimensional boson operators replacing the finite-dimensional spin operators. The values of the first three coefficients in series (2) and (11), calculated in spin-wave theory,[16–18] have been confirmed[21] later by a computation of the zero-loop and one-loop corrections to the free energy and magnetization in a spin-operator scheme, i.e., without bosonization. Hence, the "nonphysical" states of H_{DM} do not contribute to the values of the first three coefficients in (2) and (11). Based on the consideration given in Ref. 3 no essential contribution of the "nonphysical" states to the fourth coefficients in (2) and (11) may be expected. It will be interesting to check this expectation by one (in our opinion) rather nontrivial investigation of two-loop corrections to the free energy and the magnetization in the spin-operator scheme.

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