# Variational bound for the energy of two-dimensional quantum antiferromagnet

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(Submitted 23 March 1993; resubmitted 20 May 1993)
Pis'ma Zh. Eksp. Teor. Fiz. **57**, No. 12, 796–800 (25 June 1993)

The variational upper bound for the ground-state energy of a two-dimensional antiferromagnetic Heisenberg model on a square lattice for an arbitrary value of the anisotropy parameter was obtained using the two-dimensional generalization of the Jordan–Wigner transformation. The result can be considered as an upper bound for the perturbation theory series about the Ising limit.

At present, two dimensional quantum spin systems attract considerable attention in connection with the problem of high-$T_c$ superconductivity. At certain values of the anisotropy parameter for the antiferromagnetic Heisenberg model the existence of the long-range order was proved.[1] However, the exact ground state is not known. In addition to the linear spin wave theory,[2] various methods of evaluating the ground state energy of the Heisenberg antiferromagnet were proposed. The perturbation theory and the cluster expansion about the Ising limit, for example, were used in Ref. 3.

However, although the convergence of the series of the perturbation theory is good, these estimates are not the variational estimates. At the same time, the energy corresponding to any reasonable variational ground-state wave function cannot be computed exactly (for example, these calculations are given in Ref. 4). Finally, the accuracy of the numerical simulations[5] at present is not sufficiently high. In this context, the variational estimates of the ground state energy for the two-dimensional antiferromagnetic Heisenberg model are of interest.

In the present letter we obtain the exact upper bound for the ground-state energy of the $s=1/2$ quantum antiferromagnet for an arbitrary value of the anisotropy parameter. Our variational estimates are sufficiently low and may be useful in connection with the study of two-dimensional spin models in the framework of the other methods.

Our method is based on the transformation which changes the statistics of particles on a two-dimensional lattice. There are several ways to define the Hamiltonian of particles which obeys the fractional statistics (anyons) on a lattice (for example, see Ref. 6). We can use the most natural form of the definition of anyon operators in terms of the fermions

$$b_i^+(\alpha)=a_i^+\exp\left(-i\alpha\sum_{l\neq i}\phi_{il}\,n_l\right),\quad n_l=a_l^+a_l, \tag{1}$$

where the operators $a_i^+$ and $a_i$ obey the Fermi statistics, and $\phi_{il}$ is the angle between the direction from the site $i$ to the site $l$ and a fixed direction, the $x$ axis, for example.

  

In accordance with the multivaluedness of the anyon wave function, the operator $b_i^+(\alpha)$ is multiple-valued at an arbitrary fractional value of the statistical parameter $\alpha$, which describes in Eq. (1) the deviation from the Fermi statistics. In particular, at $\alpha=1$ the operators (1) are the hard-core boson operators, which commute at different sites and behave like the fermions at the same site. Expressing the spin operators ($s=1/2$) in terms of the Holstein–Primakoff boson operators

$$S_i^+=b_i^+, \quad S_i^-=b_i, \quad S_i^z=b_i^+b_i-\frac{1}{2},$$

we obtain the representation of spin operators in terms of the fermions which can be thought of as a two-dimensional generalization of the standard Jordan–Wigner transformation for one dimension:

$$S_i^+=a_i^+\exp\left(-i\sum_{l\neq i}\phi_{il}n_l\right), \quad S_i^z=a_i^+a_i-\frac{1}{2}.$$

The Hamiltonian of the Heisenberg antiferromagnet $H=\Sigma_{\langle ij\rangle}S_iS_j$ has a complicated form

$$H=-\frac{1}{2}\sum_{\langle ij\rangle}\left[a_i^+a_j\exp\left(-i\sum_{l\neq i,j}\phi_{ijl}n_l\right)+\text{H.c.}\right]+\sum_{\langle ij\rangle}\left(n_i-\frac{1}{2}\right)\left(n_j-\frac{1}{2}\right), \quad (2)$$

where $\phi_{ijl}=\phi_{il}-\phi_{jl}$, and $\langle ij\rangle$ denotes the nearest-neighbor sites. The minus sign in front of the first term in Eq. (2) is due to the redefinition of the operators $a_i\rightarrow -a_i$ on one of the sublattices of the square lattice. In order to simplify the Hamiltonian, we can make the substitution $n_l\rightarrow\bar{n}_l$ in the exponential of Eq. (2), where $\bar{n}_i$ is the average particle number at a given site, $\bar{n}=1/2$ for the half filling ($S^z=0$), which will be considered in the present paper. This procedure is usually referred to as a (vector) mean-field (MF) approximation. After this substitution the MF Hamiltonian

$$H_{\text{MF}}=-\frac{1}{2}\sum_{\langle ij\rangle}(\chi_{ij}a_i^+a_j+\text{H.c.})+U\sum_{\langle ij\rangle}\left(n_i-\frac{1}{2}\right)\left(n_j-\frac{1}{2}\right), \quad (3)$$

where $\chi_{ij}=\exp(-i\Sigma_l\phi_{ijl}\bar{n}_l)$, describes the system of fermions in a uniform statistical magnetic field of magnitude corresponding to the flux $\phi=\pi$ through the plaquette. The parameter $U=1$ for the isotropic model. Because of the gauge invariance [$a_i\rightarrow a_i\exp(\theta_i)$], the phases of $\chi_{ij}$ depend on the gauge-fixing condition. The sum of the phases near the closed contour is fixed and equal to the one-half flux quantum through the plaquette for the case of the half filling. The eigenstates of the MF Hamiltonian do not depend on the choice of the gauge. The second term in Eq. (3) is the interaction of fermions.

We used the variational theorem, proved in Ref. 7 for the hard-core bosons in the absence of the interaction term. Let $\psi_{\text{MF}}(i_1,...,i_N)$ and $E_{\text{MF}}$ be respectively the exact ground-state wave function and the ground-state energy of the MF Hamiltonian (3) ($i_1,...,i_N$ are the particle positions, $\langle\psi_{\text{MF}}|\psi_{\text{MF}}\rangle=1$). Consider the contribution of a given bond to the expectation value of Eq. (3) over the ground state. We have the following inequality:

$$-\sum_{i_2,\ldots,i_N}|\psi_{\mathrm{MF}}(i,i_2,\ldots,i_N)|\,|\psi_{\mathrm{MF}}(j,i_2,\ldots,i_N)|$$

$$\leqslant -\mathrm{Re}\left(\sum_{i_2,\ldots,i_N}\psi^*_{\mathrm{MF}}(i,i_2,\ldots,i_N)\psi_{\mathrm{MF}}(j,i_2,\ldots,i_N)\right).$$

The left-hand side of this inequality is the contribution to the expectation value of the exact Hamiltonian (2) in the bosonic representation. The normalization and the expectation value of the operator, given by the last term in Eq. (3), are the same for the wave functions $\Psi_{\mathrm{MF}}$ and $|\Psi_{\mathrm{MF}}|$. We thus proved that the ground-state energy of the initial bosonic Hamiltonian $E_0$ is bounded from above by $E_{\mathrm{MF}}$:

$$E_0 \leqslant E_{\mathrm{MF}}.$$

This relation allows us to obtain an upper bound for the energy of an antiferromagnet. We must obtain an appropriate *variational* estimate for the ground-state energy of the MF Hamiltonian (3). As a variational wave function let us choose the wave function corresponding to the Hamiltonian which is obtained from $H_{\mathrm{MF}}$ in the mean-field approximation with respect to the fermion interaction. We assume that the Néel order exists in this state. Linearizing the interaction and using the substitution $\langle n_i\rangle \to (-1)^i\Delta/4$ [we use the notation $(-1)^i=(-1)^{i_z+i_y}$], we obtain the Hamiltonian

$$-\frac{1}{2}\sum_{\langle ij\rangle}(\chi_{ij}a_i^+a_j+\mathrm{H.c.})-\Delta\sum_i(-1)^i n_i. \tag{4}$$

In this formula $\Delta$ is the variational parameter which will be determined from the condition of minimum of the expectation value of $H_{\mathrm{MF}}$ in the state given by the ground state of the mean-field Hamiltonian [Eq. (4)]. This expectation value is the variational bound for the energy $E_{\mathrm{MF}}$. Note that the choice of the wave function is consistent with the MF treatment of the statistical interaction, since the sum of the phases near the plaquette for the Néel ordered state is the same as in the case $\bar{n}_i=1/2$.

The calculations can be easily performed using the symmetric gauge

$$\chi_{i,i+\hat{x}}=\frac{1}{\sqrt{2}}\,[1+i(-1)^i],\quad \chi_{i,i+\hat{y}}=\frac{1}{\sqrt{2}}\,[1-i(-1)^i],$$

where $\hat{x}$ and $\hat{y}$ are the unit vectors corresponding to the lattice spacing. In the momentum space in terms of the doublets $\psi_{1k}=(a_k,\ a_{k-Q})$ $[0<k_x,\ k_y<\pi,\ Q=(\pi,\pi)]$ and $\psi_{2k}=(a_k,\ a_{k-Q_1})$ $[0<-k_x,\ k_y<\pi,\ Q_1=(-\pi,\pi)]$ Eq. (4) has the form

$$H=\sum_{k_x>0,\ k_y>0}\psi^+_{1k}M_k\psi_{1k}+\sum_{k_x<0,\ k_y>0}\psi^+_{2k}M_k\psi_{2k},$$

where the matrix $M_k$ is

$$M_k=-\begin{pmatrix}c_1 & \Delta-ic_2\\ \Delta+ic_2 & -c_1\end{pmatrix},\quad c_{1,2}=\frac{1}{\sqrt{2}}\,(\cos k_x\pm\cos k_y).$$

The eigenvalues are $E_k = \pm(\cos^2 k_x + \cos^2 k_y + \Delta^2)^{1/2}$, where the momentum $k$ is restricted to the half of the Brillouin zone, $k_y > 0$. The negative energy levels are filled. Let us calculate the average of $H_{\mathrm{MF}}$ over this state. The values of $\langle \chi_{ij} a_i^+ a_j \rangle$ for a given $\langle ij \rangle$ do not depend on the choice of the gauge. These values are real (and positive) and can be deduced from the parity invariance of our state. The expectation value of the second term in Eq. (3) is $\langle n_i n_j \rangle = \langle n_i \rangle \langle n_j \rangle - \langle a_i^+ a_j \rangle \langle a_j^+ a_i \rangle$. The expression for the particle number at a given site has the form $\langle n_i \rangle = 1/2 + (-1)^i \Delta_1/4$, where the parameter $\Delta_1$ does not coincide with the parameter $\Delta$. We obtain for $\Delta_1$ and $\xi = |\langle a_i^+ a_j \rangle|$ (which is the same for all bonds) the following expressions:

$$\Delta_1 = 8 \sum_{k_x>0,\ k_y>0} \frac{\Delta}{E_k}, \quad \xi = \sum_{k_x>0,\ k_y>0} \frac{\cos^2 k_x + \cos^2 k_y}{E_k}.$$

The final expression for the variational estimate is

$$\frac{E^{\mathrm{var}}}{2L^2} = \frac{\Delta^2}{16U} - \sum_{k_x>0,\ k_y>0} E_k - \frac{U}{16}\left(\Delta_1 - \frac{\Delta}{U}\right)^2 - \xi^2, \tag{5}$$

where $L^2$ is the number of sites. The sum of the first two terms is the energy in the mean-field approximation [Eq. (4)].

At $U=0$, we obtain the exact energy of the MF Hamiltonian, and the corresponding estimate of the energy for the XY model is $-0.2395$ per bond. In comparison with the energy determined with the help of numerical simulations[5] $-0.27(\pm 10\%)$, the bound is too high. This bound is less restrictive than the bound based on the simple trial variational wave function. For example, the energy corresponding to the Néel ordered state (in the $y$ direction) is $-0.25$. This value is in agreement with the assertation in Refs. 7 and 8 that the corrections due to the fluctuations near the average magnetic field background are on the order of unity. The situation is different for the isotropic (XXX) model ($U=1$). In this case the perturbation theory series rapidly converges and the corrections due to the statistics of particles are suppressed. For the Hamiltonian (2), for example, the corrections to the MF approximation are on the order of $\sim 1/(2U)^6$, which is a sufficiently small value.[8] In this sense, our result can be considered as an estimate of the upper bound for the perturbation theory series about the Ising limit. It is difficult to establish restrictions of this type by using other methods. Minimizing expression (5) with respect to $\Delta$ ($\Delta_0 = 1.19$), we obtain $E_{xxx}^{\mathrm{var}}/2L^2 = -0.33034$, which is a sufficiently good upper bound for the energy. For comparison, the best estimate obtained using the method of Ref. 3 is $-0.334$. Note that although the prediction of the linear spin wave theory[2] is $-0.329$, this method does not result in the correct ground-state wave function and this value cannot be considered as a variational bound.

For the anisotropic model we proceed as follows. For simplicity, let us consider the axially symmetric model, although our method can be easily generalized to the case of arbitrary asymmetry. We use the description in terms of the Holstein–Primakoff bosons for the equivalent Hamiltonian $H = \Sigma_{\langle ij \rangle}(S_i^x S_j^x + \gamma S_i^y S_j^y + S_i^z S_j^z)$. After the substitution $b_i \to (-1)^i b_i$ we obtain

$$H=-\sum_{\langle ij\rangle}\left(\frac{1+\gamma}{4}\,(b_i^+ b_j+\text{H.c.})+\frac{1-\gamma}{4}\,(b_i^+ b_j^+ +\text{H.c.})\right)+\sum_{\langle ij\rangle}\left(n_i-\frac{1}{2}\right)\left(n_j-\frac{1}{2}\right). \tag{6}$$

Consider the trial variational wave function with a fixed number of bosons. For this state the expectation value of the second term $\sim(b_i^+ b_j^+ + b_i b_j)$ in Eq. (6) is zero. The Hamiltonian (6), without this term, can be used to obtain a variational estimate for the ground-state energy of arbitrary $\gamma$ according to our method. Note that the contribution of the omitted term is small in the framework of the perturbation theory[3] since it appears only in the fourth order. The analysis can be performed at an arbitrary value of the parameter $\gamma$. For the XY model ($\gamma=0$), which is equivalent to a system of hard-core bosons at the half filling, we found the estimate $-0.26776$ per bond ($\Delta_0=3.4$). This estimate is in agreement with the result of numerical simulations.[5]

In conclusion, although the wave function corresponding to the mean-field Hamiltonian (3) cannot be used to describe the long-range properties of the model (for example, the energy of the low-lying excitations), the ground-state energy can be estimated with a sufficiently high accuracy. We found the *variational* upper bound for the ground-state energy of the two-dimensional Heisenberg antiferromagnet on a square lattice at arbitrary value of the anisotropy parameter. Our results can be thought of as a peculiar upper bound for the perturbation theory series about the Ising limit. These results may be useful in the context of the other approaches.

This work was supported, in part, by a Soros Foundation Grant awarded by the American Physical Society.

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Published in English in the original Russian journal