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VARIATIONAL BOUND FOR THE ENERGY OF TWO-DIMENSIONAL QUANTUM ANTIFERROMAGNET

A.A.Ovchinnikov

Institute for Nuclear Research of the Russian Academy of Sciences,
117312 Moscow, Russia

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

At present time two dimensional quantum spin systems attract much attention in connection with the problem of high-T_c superconductivity. For the antiferromagnetic Heisenberg model at some values of the anisotropy parameter the existence of the long-range order was proved [1], however the exact ground state is not known. Apart from the linear spin wave theory [2] various methods to evaluate the ground state energy for the Heisenberg antiferromagnet were proposed. For instance the perturbation theory and the cluster expansion about the Ising limit were used [3]. However, although the convergence of the series of the perturbation theory is good these estimates are not the variational ones. At the same time the energy corresponding to any reasonable variational ground-state wave function cannot be computed exactly (for example of these calculations see ref.[4]). Finally at present time the accuracy of the numerical simulations [5] 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 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 change the statistics of particles on a two-dimensional lattice. There are several ways to define the Hamiltonian of particles obeying 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

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

where the operators a_i^+, a_i obeys Fermi statistics and ϕ_{il} is the angle between the direction from the site i to the site l and some fixed direction, x-axis for example. In accordance with the multi-valuedness of the anyon wave function the operator $b_i^+(\alpha)$ is multi-valued at arbitrary fractional value of the statistical parameter α, 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 bose 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 well known 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 $H = \sum_{<ij>} \mathbf{S}_i \mathbf{S}_j$ has a complicated form

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

where $\phi_{ijl} = \phi_{il} - \phi_{jl}$ and $< ij >$ denotes the nearest neighbour sites. The minus sign before the first term in Eq.(2) is due to the redefinition of the operators $a_i \to -a_i$ on one of the sublattices of the square lattice. In order to simplify the Hamiltonian one can make the substitution $n_l \to \bar{n}_l$ 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 refered to as a (vector) mean field (MF) approximation. After this substitution the MF Hamiltonian

$$H_{\text{MF}} = -\frac{1}{2} \sum_{<ij>} (\chi_{ij} a_i^+ a_j + \text{h.c.}) + U \sum_{<ij>} (n_i - \frac{1}{2})(n_j - \frac{1}{2}), \quad (3)$$

where $\chi_{ij} = \exp(-i \sum_l \phi_{ijl} \bar{n}_l)$, describes the system of fermions in the homogeneous statistical magnetic field with the magnitude corresponding to the flux $\phi = \pi$ through the plaquette. The parameter $U = 1$ for the isotropic model. Due to the gauge invariance ($a_i \to a_i \exp(\theta_i)$) the phases of χ_{ij} are depend on the gauge fixing condition. The sum of the phases around 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 does not depend on the choice of the gauge. The second term in Eq.(3) is the interaction of fermions.

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

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

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

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 as well as the expectation value of the operator given by the last term of Eq.(3) are the same for the wave functions Ψ_{MF} and $|\Psi_{\mathrm{MF}}|$. Thus it is proved that the ground-state energy of the initial bosonic Hamiltonian E_0 is bounded from above by E_{MF}:

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

This relation allows one to obtain an upper bound for the energy of the antiferromagnet. We have to obtain the 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_{MF} in the mean field approximation in respect to the fermion interaction. We assume the existence of Neel order in this state. Linearising the interaction and using the substitution $< n_i > \to (-1)^i\Delta/4$ (we use the notation $(-1)^i = (-1)^{i_x+i_y}$) we obtain the Hamiltonian

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

In this formula Δ is the variational parameter which is to be determined from the condition of minimum of the expectation value of H_{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_{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 around the plaquette for the Neel ordered state is the same as in the case of $\bar{n}_i = 1/2$.

The calculations are most easily performed using the symmetric gauge

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

where $\hat{x}, \hat{y}$ 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 $\psi_{2k} = (a_k, a_{k-Q_1})$ $(0 < -k_x, k_y < \pi,$ $Q_1 = (-\pi,\pi))$ the equation (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

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

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 Broullien zone $k_y > 0$. The negative energy levels are filled. Let us calculate the average of H_{MF} over this state. The values of $< \chi_{ij}a_i^+a_j >$ for a given $< ij >$ does not depend on the choice of the gauge. This values are real (and positive) which can be deduced from the parity invariance of our state. The expectation value of the second term in Eq.(3) is $< n_i n_j >=< n_i >< n_j > - < a_i^+ a_j >< a_j^+ a_i >$. The expression for the particle number at a given site has the form $< n_i >= 1/2 + (-1)^i \Delta_1/4$, where the parameter Δ_1 does not coincide with the parameter Δ. We obtain for Δ_1 and $\xi = | < a_i^+ a_j > |$ (which is the same for all bonds) the following expressions:

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

The final expression for the variational estimate is

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

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 get the exact energy of the MF Hamiltonian and the corresponding estimate for the energy for the XY model is -0.2395 per bond. In comparison with the energy determined with the help of the numerical simulations $-0.27(\pm 10\%)$ [5], the bound is too high. It is less restrictive than the bound based on the simple trial variational wave function, For example the energy corresponding to the Neel ordered state (in the y-direction) is -0.25. That is in agreement with the statement of ref's.[7,8] that the corrections due to the fluctuations around the average magnetic field background are of order of unity. The situation is different for the isotropic (XXX) model ($U = 1$). In this case the perturbation theory series is rapidly converges and the corrections due to the statistics of particles are suppressed. For instance for the Hamiltonian (2) the corrections to the MF approximation are of order $\sim 1/(2U)^6$ which is a sufficiently small value [8]. In this sense our result can be considered as an estimate from above for the perturbation theory series about the Ising limit. It is difficult to establish the restrictions of this type using the other methods. Minimizing the expression (5) with respect to Δ ($\Delta_0 = 1.19$) we obtain $E^{var}_{xxx}/2L^2 = -0.33034$, which is 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 $H = \sum_{<ij>} (S_i^x S_j^x + \gamma S_i^y S_j^y + S_i^z S_j^z)$. After the substitution $b_i \to (-1)^i b_i$ we get

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

Consider the trial variational wave function with the 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 the variational estimate for the ground-state energy for arbitrary γ 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 arbitrary value of the parameter γ. For the XY model ($\gamma = 0$) which is equivalent to the system of the 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 result of the 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 the 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 and may be useful in the context of the other approaches.

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