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Andrzej M Oleś† and Barbara Oleś‡

† Institute of Physics, Jagellonian University, Reymonta 4, PL-30-059 Kraków, Poland
‡ Institute of Physics, Technical University of Kraków, Podchorążych 2, PL-30-084 Kraków, Poland

Abstract. The variational wave function proposed by Bartkowski to treat the ground state of a quantum antiferromagnet is generalized to arbitrary spin. We derive the fundamental equations of this method for the energy and magnetization by using a local cluster expansion. The leading order corrections to the wave function in the limit of either large spin S or lattice dimension D are identified. The good quality of the wave function is confirmed by the ground state energy of $E_0 = -0.3340J$ obtained for the Heisenberg $S = \frac{1}{2}$ antiferromagnet on the square lattice. We present results obtained for the system of two planes and for three-dimensional SC and BCC lattices, as well as for the three-dimensional anisotropic Heisenberg model. It is found that the quantum fluctuations in a two-plane system are already closer to a three-dimensional than to a two-dimensional antiferromagnet, while a weak interplane coupling in the latter case hardly influences the nearest-neighbour spin correlations within the planes.

1. Introduction

The discovery of high-temperature superconductors with their two-dimensional (2D) CuO_2 planes, which exhibit a quasi-2D antiferromagnetic (AF) order in the undoped systems [1,2] caused a renewed interest in the 2D Heisenberg model. It is well known that the model is exactly solvable in one dimension, with the exact ground state energy of $-0.4419J$ per bond [3], where J is the exchange interaction, and exhibits no AF long-range order. While the existence of the AF long-range order in a three-dimensional (3D) system was proved rigorously by Kennedy, Lieb and Shastry [4], the issue was controversial for a 2D system due to the theorem of Mermin and Wagner [5]. Numerous studies undertaken recently by various powerful analytic and numerical methods have demonstrated that the long-range AF order exists in a 2D Heisenberg model at temperature $T = 0$ [6]. Although there is no exact solution in two dimensions, the calculations performed within the Green function Monte Carlo method provided a very accurate estimate for the ground state energy of $-(0.3347 \pm 0.0002)J$ per bond [7–9]. This result is consistent with the energy of $-(0.334 \pm 0.001)J$ obtained by Huse [10] from the series expansion derived earlier by Parrinello and Arai [11], as well as with the more accurate estimation of $-(0.3348 \pm 0.0003)J$ found recently by Singh [12] from the expansion around the Ising limit. Similar, but slightly higher values of energy were obtained by various analytic and numerical methods [6]. We will not attempt to improve these results for the 2D Heisenberg model, but instead we want to present a simple variational approach that gives results of comparable quality. Its conceptual and numerical simplicity allows us to estimate the energy

of Heisenberg antiferromagnets on different lattices in a very fast and efficient way, as we demonstrate below.

Numerical methods usually give little insight into the nature of the ground state wave function and the way it could be treated approximately in an analytic approach. Therefore, analytic, and in particular variational, approaches are very useful as they allow not only for a more transparent description of the Heisenberg magnets, but also contribute to better understanding of the nature and role played there by quantum fluctuations. The conceptually simplest approach starts from the spin density wave solution of the Hubbard model, which is variationally improved with the help of the Gutzwiller *ansatz* [13]. The energy obtained in this way by Yokoyama and Shiba [13] of $-0.321J$ lies well above the other estimates as this variational *ansatz* implements only the local constraint and neglects the short-range correlations. They are included in two variational wave functions widely used for a Heisenberg antiferromagnet. The first of them, proposed by Marshall in 1955 [14], focuses on the statistical distribution of spins over the lattice and optimizes the distance dependence of the spin–spin correlation function $\langle S_i^z S_j^z \rangle$ [14–16]. It gives a rigorous variational upper bound for the ground state energy of a 2D antiferromagnet of $-0.3319J$ [15]. The second wave function was proposed by Bartkowski in 1972 [17]. It implements the quantum fluctuations on the bonds in the classical Néel state. Unfortunately, it was claimed in the original paper that it gives a ground state energy only of $-0.329J$ per bond which is certainly worse than any other approach to the Heisenberg Hamiltonian that includes the quantum fluctuations, except perhaps for the lowest-order spin wave theory result [18]. Therefore, the Bartkowski wave function was neglected for a long time until one of us demonstrated that the quality of this wave function is *de facto* much better [19], provided that the fully self-consistent minimization of the obtained expression for the ground state energy is performed. The method proposed originally by Bartkowski then gives the energy of $-0.3320J$ [19] instead of $-0.329J$ [17]. Therefore, we use this wave function in the present contribution as a conceptually simple method to investigate the quantum fluctuations in the following systems: (i) diamond lattices in D dimensions; (ii) the anisotropic Heisenberg model in two and three dimensions, 3D and for the system of two planes; and, finally, (iii) for the anisotropic 3D Heisenberg model with a weaker exchange interaction between the 2D planes than within them.

2. The variational wave function and the calculation method

In order to demonstrate the role of quantum fluctuations in the reduction of the ground state energy we consider the anisotropic Heisenberg model on bipartite lattices

$$H_J = J \sum_{\langle ij \rangle} \left(\frac{\gamma}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + S_i^z S_j^z \right) \tag{1}$$

where J is the exchange interaction between the nearest-neighbour spins S, and the anisotropy parameter γ stands for the ratio of the exchange parameters in the quantum fluctuation, i.e. $\sim (S_i^+ S_j^- + S_i^- S_j^+)$ part, and in the Ising part, respectively. The Hamiltonian (1) gives the Ising and Heisenberg Hamiltonians for $\gamma = 0$ and 1, respectively. The classical ground state of (1), which becomes exact in the Ising limit, is the Néel state

$$|\psi_N\rangle = \prod_{i \in A} a_{i\uparrow}^\dagger \prod_{j \in B} a_{j\downarrow}^\dagger |0\rangle \tag{2}$$

written here by using fermion creation operators, $a_{i\uparrow}^\dagger$ and $a_{i\downarrow}^\dagger$ for the sublattices A and B, respectively. Bartkowski's idea was to correct this classical state by allowing for the

reversals of pairs of the nearest-neighbour spins, i.e. two spins terminating a particular bond in the lattice. The variational wave function is therefore of the form [17]

$$|\phi_0\rangle = \prod_{i\in A,\delta(i)} \left(1 + \alpha\frac{S_i^- S_{i+\delta}^+}{2S}\right)^{2S} |\psi_N\rangle \tag{3}$$

where $i + \delta(i)$ stands for a neighbour of site i. This wave function may be used for any spin S, as the $2S$ factors $(1 + \alpha S_i^- S_{i+\delta}^+/2S)$ for each bond allow us to completely reverse the spins. In the original wave function [17] only one such factor per bond was included which allows for a single quantum fluctuation and is therefore appropriate only for $S = \frac{1}{2}$. In the applications of the wave function (3) we shall limit ourselves to the most interesting case of $S = \frac{1}{2}$.

The variational parameter α has to be determined from the minimization of the ground state energy

$$E_0 = \frac{\langle\phi_0|H_J|\phi_0\rangle}{\langle\phi_0|\phi_0\rangle}. \tag{4}$$

It may be easily verified that the wave function (3) reproduces the exact singlet wave function for a pair of spins $S = \frac{1}{2}$ with the choice of $\alpha = 1$ [19]. The form of this wave function (3) resembles the Gutzwiller *ansatz* for the Hubbard model [20]. Both wave functions emphasize *local* correlations of certain kind, but the latter wave function implements the correlations in a Slater determinant, while the former implements quantum fluctuations into the classical AF state of (already) localized fermions. As for the Gutzwiller wave function, in the present case one may also propose a combinatorial way of calculating various average quantities [17,21]. We have chosen to use a certain generalization of the original approximate method as proposed by Bartkowski which is based on a local cluster expansion [19].

In order to calculate the energy of the ground state, one has to evaluate the ground state energy E_0 which could be calculated exactly from equation (4) only for small finite clusters. As for the infinite system the exact evaluation of its energy is not possible, one includes only the connected diagrams up to a given order in the variational parameter α, and evaluates the energy per bond according to the formula

$$E_0 = J\frac{\langle\phi_0|(\gamma/2)(S_0^+ S_a^- + S_0^- S_a^+) + S_0^z S_a^z|\phi_0\rangle_c}{\langle\phi_0|\phi_0\rangle_c} \tag{5}$$

where $(0, a)$ is an arbitrary bond and $\langle...\rangle_c$ means that only connected diagrams are included in the numerator and the denominator of equation (5). The quantum fluctuations, $\sim S_i^- S_j^+$, which result from the expansion of $\langle\phi_0|$ and $|\phi_0\rangle$, are represented there as lines in a connected diagram. Of course, the energy calculated in this way is not exact for the wave function (3) used and thus equation (5) has to be treated as a variational *ansatz*. In the contribution from the $(0, a)$ bond one includes explicitly the quantum fluctuations of the spins at sites 0 and a. In contrast, the quantum fluctuations on the neighbouring sites are only partially included, i.e. only for those bonds that connect this site with the central sites 0 or a. Therefore, one encounters the problem of how to include the effect of quantum fluctuations on those (outside) bonds not explicitly treated within the performed cluster expansion, i.e. how the considered cluster should be embedded in order to simulate an infinite system. Consider a bond $(0, a)$ for which the energy is calculated according to equation (4). The bonds not treated explicitly by the included quantum fluctuations reduce the probability that these quantum fluctuations can occur and that any of the considered diagrams is successfully completed. This effect may be included in a statistical way by introducing a probability

P that a particular spin is already reversed due to the other $(z-1)$ outside bonds [17]. It is related to the probability Q that any spin in the lattice is not affected by the quantum fluctuations at all z bonds,

$$P^z = Q^{(z-1)} \tag{6}$$

where z is the number of nearest neighbours in the considered lattice. By construction, the latter probability is related to the *local* reduction of staggered magnetization due to quantum fluctuations. For a general spin S one finds that

$$\langle S_0^z \rangle = \frac{2S+1}{2} Q - \frac{1}{2} \tag{7}$$

which generalizes the respective relation given by Bartkowski for $S = \frac{1}{2}$ [17]. Thus, one needs the probability P (or Q) in order to perform the minimization of the ground state energy, E_0. This probability may be determined from the equation for the average magnetic moment, $\langle S_0^z \rangle$, calculated again by making use of the linked cluster theorem (here we assume that site $0 \in A$)

$$\langle S_0^z \rangle = \frac{\langle \phi_0 | S_0^z | \phi_0 \rangle_c}{\langle \phi_0 | \phi_0 \rangle_c}. \tag{8}$$

Again, equation (8) is an *ansatz* consistent with the expansion (5) performed for the ground state energy. In the linked cluster expansion one finds that the contributions to the matrix elements $\langle \phi_0 | S_0^z | \phi_0 \rangle$ and $\langle \phi_0 | \phi_0 \rangle$ come either from self-retracing paths, or from closed loops (if such loops exist in the considered lattice). Examples of such closed loops in a 2D system were given in [19], and more details are given in the appendix. By the evaluation of these matrix elements one finds for $S = \frac{1}{2}$

$$\langle S_0^z \rangle = \left(S_0^z + z\alpha^2 (S_0^z - 1) P + zK(S_0^z - 1) \sum_{k=2}^n c_{2k} \alpha^{2k} P^{2k-3} \right)$$

$$\times \left(1 + z\alpha^2 P + zK \sum_{k=2}^n c_{2k} \alpha^{2k} P^{2k-3} \right). \tag{9}$$

Here S_0^z is the average magnetization in the Néel state $|\psi_N\rangle$, while K is the number of non-equivalent closed loops of length four bonds, built around a single bond, as introduced in the appendix. Finally, c_{2n} are the combinatorial coefficients that express the number of non-equivalent loops built by n bonds. By definition $c_4 = 1$, while $c_6 = 3$, 6, and 9 for a 2D square lattice, the system consisting of two parallel planes, and for both 3D lattices (SC and BCC), respectively. We have also used below $c_8 = 10$ for the 2D square lattice. By combining (6), (7), and (9), one finds the following equation for P, which we reproduce here only for $S = \frac{1}{2}$:

$$P^{z/(z-1)} \left(1 + z\alpha^2 P + zK \sum_{k=2}^n c_{2k} \alpha^{2k} P^{2k-3} \right) = 1. \tag{10}$$

This may be solved for any given value of α. Equation (10) reproduces the respective condition for P used by Bartkowski [17], if the contribution from closed loops is neglected, i.e. at $K = 0$.

The next step is the calculation of energy from equation (5). The structure of the contributions from the Ising part of the Heisenberg Hamiltonian (1) is different from that of the contributions that result from a quantum fluctuation $\sim S_0^- S_a^+$ on the considered bond (0–a). As the quantum fluctuations in $\langle \phi_0 | H_J | \phi_0 \rangle_c$ must be compensated pairwise, in the first

case one has to include an even number of quantum fluctuations from the wave functions $\langle\phi_0|$ and $|\phi_0\rangle$, while this number has to be odd in one of these wave functions in the second case. As a result one finds (see the appendix for more details) that

$$E_0 = -\frac{J}{4}\frac{1 + \alpha^2[1 - 2(z-1)P] + \alpha^4(z-1)^2P^2 - 4\gamma\alpha + (\alpha^2 - 4\alpha\gamma)KW}{1 + \alpha^2[1 + 2(z-1)P] + \alpha^4(z-1)^2P^2 + \alpha^2KW} \tag{11}$$

where

$$W = K\sum_{k=2}^{n}c_{2k}\alpha^{2k-2}P^{2k-2}. \tag{12}$$

Next, the ground state energy E_0 has to be minimized with respect to the value of the variational parameter α. In the limit of low density of spin deviations from the Néel state, i.e. if the quantum fluctuations are independent of each other, one finds for an AF Heisenberg model with spin S that [17]

$$\alpha = -S/(2Sz - 1). \tag{13}$$

This value of α, obtained from E_0 by taking only the contributions up to $\sim \alpha^2$ and assuming that $P = 1$, may be considered to be the lowest-order approximation; the improved value of α may be found by numerical minimization of the energy E_0, as given by equation (11). This minimization procedure has to be performed self-consistently with equation (10), which gives the value of P for a given α. More details concerning the derivation of (10) and (11) may be found in [17] and [19].

Once the values of α and P are known, one may calculate the order parameter $\langle S_0^z\rangle$ and the ground state energy E_0. We have quantified the quantum correction to the classical (or mean field) ground state energy of an $S = \frac{1}{2}$ antiferromagnet, $E_{\text{MF}} = -J/4$, by

$$\delta = \frac{E_{\text{MF}} - E_0}{|E_{\text{MF}}|}. \tag{14}$$

The variational wave function (3) also allows for the calculation of the nearest-neighbour correlation function $\langle S_1^z S_2^z\rangle$, which provides information about the short-range order in the ground state. By using the same local cluster expansion as for the calculation of energy (11) one finds that

$$\langle S_1^z S_2^z\rangle = -\frac{1}{4}\frac{1 + \alpha^2[1 - 2(z-1)P] + \alpha^4(z-1)^2P^2 + \alpha^2KW}{1 + \alpha^2[1 + 2(z-1)P] + \alpha^4(z-1)^2P^2 + \alpha^2KW}. \tag{15}$$

In section 3 we present the numerical results for the $S = \frac{1}{2}$ AF Heisenberg model defined on several lattices.

In a similar way we investigated an anisotropic 3D cubic lattice with stronger exchange interaction $J_\parallel$ in the planes, and weaker interaction $J_\perp$ between them, described by the Hamiltonian of the form

$$H = J_\parallel \sum_{n,\langle ij\rangle}\left(\frac{1}{2}\big(S_{ni}^+ S_{nj}^- + S_{ni}^- S_{nj}^+\big) + S_{ni}^z S_{nj}^z\right)$$

$$+ J_\perp \sum_{n,i}\left(\frac{1}{2}\big(S_{ni}^+ S_{n+1,i}^- + S_{ni}^- S_{n+1,i}^+\big) + S_{ni}^z S_{n+1,i}^z\right). \tag{16}$$

It is convenient to introduce the anisotropy parameter $\xi = J_\perp/J_\parallel$ and label the spin operators S_{ni} by two indices, the plane index n and the intra-plane index i. The variational wave

function for the anisotropic system described by the Hamiltonian (16) may be constructed by generalizing equation (3),

$$
|\phi_0\rangle = \prod_{\langle n,i\rangle \in A, \delta(i)} \left(1 + \alpha \frac{S_{ni}^- S_{n,i+\delta}^+}{2S}\right)^{2S} \prod_{\langle n,i\rangle \in A, \rho(n)} \left(1 + \beta \frac{S_{ni}^- S_{n+\rho,i}^+}{2S}\right)^{2S} |\psi_N\rangle \tag{17}
$$

where $[n, i + \delta(i)]$ stands for a neighbour of site (n, i) in the plane n and $[n + \rho(k), i]$ is a neighbour of site (n, i) in the plane above or below the plane n. This wave function may be in principle used for any spin S, but we consider it here only for $S = \frac{1}{2}$ as in this case the quantum fluctuations are largest and this value of S is relevant for highly anisotropic exchange interactions in the high temperature superconductors.

Although the wave function (17) depends formally on two variational parameters, we adopted an *ansatz* that $\beta = \xi\alpha$. It may be easily verified that this *ansatz* includes the leading part of the energy gain resulting from the interplane quantum fluctuations and is consistent with the expansion performed in powers of α. It is then straightforward to derive the equations for $\langle S_0^z \rangle$ and E_0 by using the same expansion as described in the appendix. One finds that the probability P is found from the condition

$$
P^{z_{\text{eff}}/(z_{\text{eff}}-1)}[1 + z_{\parallel}\alpha^2 P + z_{\perp}\beta^2 P
$$
$$
+ z_{\parallel}K\alpha^2(\alpha^2 + 2\beta^2)P^3(1 + 6\alpha^2 P^2 + 3\beta^2 P^2)] = 1. \tag{18}
$$

Here the number of nearest neighbours in the plane and in the neighbouring planes is $z_{\parallel} = 4$ and $z_{\perp} = 2$, respectively, and the *effective* number of nearest neighbours is defined as $z_{\text{eff}} = z_{\parallel} + \xi z_{\perp}$. The energy of the ground state per one bond in the plane is found from the formula

$$
E_0 = J \frac{\langle \phi_0 \mid [S_{ni}^z S_{nj}^z + \frac{1}{2}(S_{ni}^- S_{nj}^+ + S_{ni}^+ S_{nj}^-)] \mid \phi_0\rangle_c}{\langle \phi_0 \mid \phi_0\rangle_c} \tag{19}
$$

where from a similar local cluster expansion to that described before one finds up to order $\sim \alpha^6$ the following matrix elements:

$$
\langle \phi_0 \mid S_{ni}^z S_{nj}^z \mid \phi_0\rangle_c = -\frac{1}{4}\{1 + \alpha^2[1 - 2(z_{\parallel} - 1)P] - 2\beta^2 z_{\perp} P
$$
$$
+ [\alpha^2(z_{\parallel} - 1) + \beta^2 z_{\perp}]^2 P^2 \tag{20}
$$
$$
+ \alpha^2(\alpha^2 + \beta^2)KP^2(1 + 6\alpha^2 P^2 + 3\beta^2 P^2)\}
$$

$$
\langle \phi_0 \mid \frac{1}{2}(S_{ni}^- S_{nj}^+ + S_{ni}^+ S_{nj}^-) \mid \phi_0\rangle_c = -\alpha[1 + (\alpha^2 + \beta^2)KP^2(1 + 6\alpha^2 P^2 + 3\beta^2 P^2)\} \tag{21}
$$

$$
\langle \phi_0 \mid \phi_0\rangle_c = 1 + \alpha^2[1 - 2(z_{\parallel} - 1)P] - 2\beta^2 z_{\perp} P + [\alpha^2(z_{\parallel} - 1) + \beta^2 z_{\perp}]^2 P^2
$$
$$
+ \alpha^2(\alpha^2 + \beta^2)KP^2(1 + 6\alpha^2 P^2 + 3\beta^2 P^2). \tag{22}
$$

The minimization of E_0 (equation (19)) over α has to be performed self-consistently with the solution of equation (18) for P, where $0 < P < 1$. With the known variational parameters α and β and the probability P we find the magnetization in the anisotropic system (15) from the equation analogous to (6), but with the replacement $z \to z_{\text{eff}}$. Finally, the nearest-neighbour spin–spin correlation function is obtained from (20) and (22),

$$
\langle S_{ni}^z S_{nj}^z \rangle = \frac{\langle \phi_0 \mid S_{ni}^z S_{nj}^z \mid \phi_0\rangle_c}{\langle \phi_0 \mid \phi_0\rangle_c}. \tag{23}
$$

3. Numerical results

Before presenting the numerical results, let us consider the limits of either $S \to \infty$, or $z \to \infty$. In both cases we are interested only in leading order corrections and thus it is sufficient to limit oneself to the terms of order $\sim \alpha^2$. One finds that for large S

$$P \simeq 1 - 4\frac{z-1}{4z+1}\frac{1}{S} \tag{24}$$

while for large z

$$P \simeq 1 - \frac{1}{2(2S+1)}\frac{1}{z}. \tag{25}$$

The expansion for large S is of less significance as it is meaningful only for $S > 1$. The region of validity of the expansion for large z is much broader. In fact, it extends down to $z \simeq 4$ for $S = \frac{1}{2}$. This can be demonstrated by minimizing the energy for a D-dimensional diamond lattice, with $z = D + 1$ and $K = 0$,

$$E_0 = -\frac{J}{4}\frac{1 + \alpha^2(1 - 2DP) + \alpha^4 D^2 P^2 - 4\gamma\alpha}{1 + \alpha^2(1 + 2DP) + \alpha^4 D^2 P^2} \tag{26}$$

for the value of P given by equation (25). For the 3D diamond lattice ($D = 3$, $z = 4$) one finds from a self-consistent solution of equations (10) and (11) the value of $P = 0.934$, while from equation (25) one finds $P = 0.953$. The detailed comparison of the numerical results for the correlation function $\langle S_1^z S_2^z \rangle$ and the quantum correction δ to the ground state energy, as defined by equation (14), obtained in the diamond lattices is given in table 1. They are compared with the results found by using the expansion for large z in figure 1. As expected, the correlation function $\langle S_1^z S_2^z \rangle$ converges to the classical limit of $\langle S_1^z S_2^z \rangle_{\text{Ising}} = -0.25$ as $z \to \infty$. Furthermore, for $z > 4$ (i.e. $D > 3$) the results of numerical minimization are practically indistinguishable from the analytic results obtained from the expansion (see figure 1). Significant corrections, both in $\langle S_1^z S_2^z \rangle$ and δ, are found only for the hexagonal lattice ($z = 3$) and for the one-dimensional (1D) chain ($z = 2$). The quantum corrections to δ the ground state energy are considerably larger there than those resulting from the large z expansion, while the short-range order, measured by the correlation function $\langle S_1^z S_2^z \rangle$, is reduced less than expected from the expansion. This may be seen as a signal that the quantum corrections to the ground state energy increase, whereas the short-range order remains well preserved, as known from the exact solution of the 1D Heisenberg chain [3].

Table 1. Variational parameter α, ground state energy E_0 per bond (in units of J) and the quantum correction δ to the ground state energy ((11), (12)), magnetic moment $\langle S_i^z \rangle$, and correlation function $\langle S_1^z S_2^z \rangle$, as obtained for diamond lattices in D dimensions. $z = D + 1$ is the number of nearest neighbours.

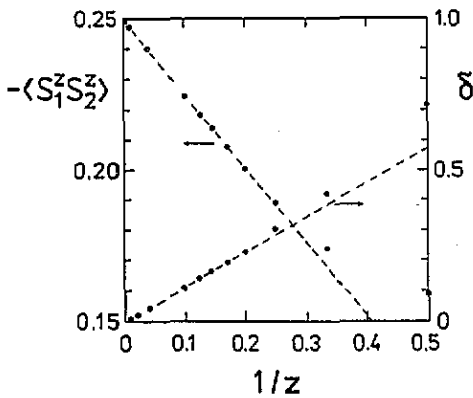| D	z	α	P	E_0	δ	$\langle S_i^z \rangle$	$\langle S_1^z S_2^z \rangle$
1	2	−0.3824	0.8907	−0.4271	0.7085	0.2933	−0.1585
2	3	−0.2285	0.9146	−0.3562	0.4248	0.3747	−0.1737
3	4	−0.1599	0.9339	−0.3252	0.3008	0.4128	−0.1890
4	5	−0.1221	0.9469	−0.3080	0.2321	0.4341	−0.2001
5	6	−0.0984	0.9559	−0.2972	0.1888	0.4474	−0.2081
6	7	−0.0825	0.9623	−0.2898	0.1590	0.4562	−0.2138
7	8	−0.0709	0.9672	−0.2843	0.1373	0.4626	−0.2183
9	10	−0.0553	0.9739	−0.2770	0.1078	0.4711	−0.2246

Figure 1. The quantum correction δ to the ground state energy and the nearest-neighbour correlation function $\langle S_1^z S_2^z \rangle$, as defined in equations (14) and (15), for diamond lattices as functions of $1/z$.
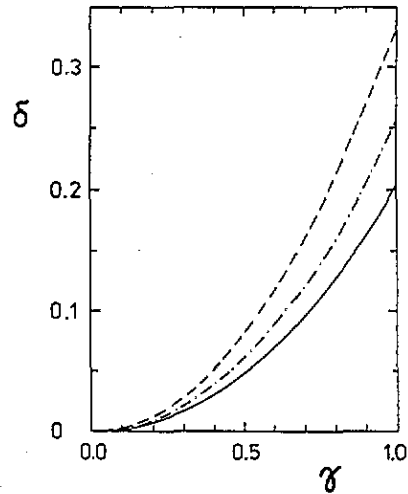
Figure 2. Quantum corrections δ to the ground state energy in the anisotropic Heisenberg model as functions of the anisotropy parameter γ. Full, dashed-dotted, and dashed lines are for the 2D square lattice, the two-plane system, and the 3D SC lattice, respectively.

Table 2. Variational parameter α, ground state energy E_0 per bond (in units of J), the quantum correction δ to the ground state energy magnetic moment $\langle S_i^z \rangle$, and correlation function $\langle S_1^z S_2^z \rangle$, as obtained for the isotropic antiferromagnetic Heisenberg model for a 2D square lattice, in the successive approximations within the local cluster expansion.

	α	E_0	δ	$\langle S_i^z \rangle$	$\langle S_1^z S_2^z \rangle$
Bartkowski method	−0.1866	−0.3320	0.3281	0.3874	−0.1724
Order ~ α^4	−0.1926	−0.3328	0.3313	0.3757	−0.1695
Order ~ α^6	−0.2010	−0.3338	0.3350	0.3656	−0.1646
Order ~ α^8	−0.2032	−0.3339	0.3356	0.3629	−0.1632
Extrapolation to α^∞	−0.2036	−0.3340	0.3358	0.3622	−0.1628

As a second application of the wave function (3) we have performed the calculations of the ground state energy E_0, magnetization $\langle S_i^z \rangle$, and the nearest-neighbour correlation function $\langle S_1^z S_2^z \rangle$ for the anisotropic Heisenberg model (1) on a 2D square lattice, the system consisting of two planes, and a 3D SC lattice. First, let us consider the case of isotropic exchange interaction. The values of energy E_0 and magnetization $\langle S_0^z \rangle$ obtained for a 2D square lattice in different orders in α, and presented in table 2, are encouraging. We note that solving self-consistently equations (25) and (32) given by Bartkowski in [17] results in a significantly better result than that originally reported, with $E_0 = -0.3320J$ and $\langle S_i^z \rangle = 0.387$ [19]. By making an expansion up to the eighth order in the variational parameter α we were able to decrease the energy down to $-0.3339J$, while the value of $\langle S_i^z \rangle$ decreases down to 0.3629. As observed in table 2, the series converges very rapidly and gives the estimated values of the energy, $E_0 = -0.3340J$ and magnetization, $\langle S_i^z \rangle = 0.3626$ for the infinite system. The value of energy obtained in this case is of very good quality indeed. It lies below the rigorous variational upper bound obtained from the other variational wave function by Huse and Elser [16] and is also better than the value of $E_0 = -0.3317J$ found by Sachdev [22] by using a different expansion. Therefore, our ground state energy
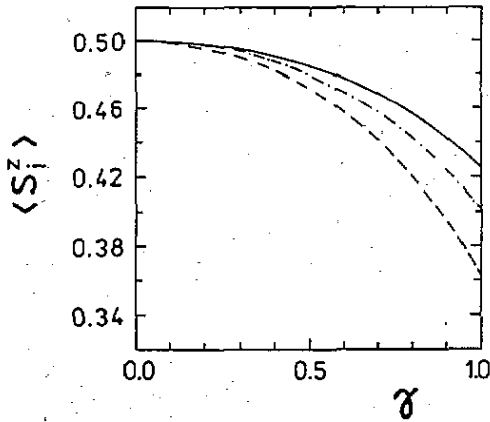
Figure 3. Order parameters $\langle S_i^z \rangle$ in the anisotropic Heisenberg model as functions of the anisotropy parameter γ. The meanings of the lines are as in figure 2.

Figure 4. Spin–spin nearest-neighbour correlation functions $\langle S_1^z S_2^z \rangle$ in the anisotropic Heisenberg model as functions of the anisotropy parameter γ. The meanings of the lines are as in figure 2.
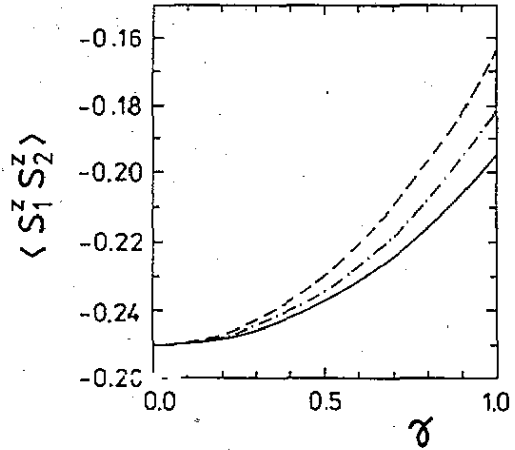
is the lowest upper bound among existing variational calculations with a *single* variational parameter. Among various analytic approaches applied so far to the AF 2D square lattice, a lower value of energy than the one found here, $E_0 = -0.3348J$, has been obtained only by Singh from the expansion around the Ising limit [12].

Table 3. Results for the variational parameter α, ground state energy E_0 per bond (in units of J), the quantum correction δ to the ground state energy magnetic moment $\langle S_i^z \rangle$, and correlation function $\langle S_1^z S_2^z \rangle$, as obtained in the expansion up to α^6 for the isotropic antiferromagnetic Heisenberg model for a 2D square lattice, two planes with the same inter- and intra-planar exchange interaction, SC and BCC lattices. z is the number of nearest neighbours and K is the number of non-equivalent closed loops, as defined in the text.

Lattice	z	K	α	P	E_0	δ	$\langle S_i^z \rangle$	$\langle S_1^z S_2^z \rangle$
Square	4	2	−0.2010	0.8955	−0.3338	0.3350	0.3656	−0.1646
Two planes	5	3	−0.1503	0.9195	−0.3142	0.2566	0.4004	−0.1806
SC	6	4	−0.1171	0.9370	−0.3015	0.2061	0.4249	−0.1940
BCC	8	12	−0.0983	0.9348	−0.2901	0.1605	0.4258	−0.1946

A similar quality of the calculated ground state energies is expected for the two-plane system and for a 3D SC lattice (see table 3). One observes that the reduction of the ground state energy due to quantum fluctuations in the two-plane system is qualitatively half way between those found in the 2D and 3D lattices. Contrary to the naive intuition, we observe that for the fixed dimension D the lattices with a higher coordination number have *lower* decrease of the ground state energy due to the quantum fluctuations on the bonds, and the *largest* energy correction due to quantum fluctuations δ is found in the diamond lattices. For instance, for $D = 3$ one finds $\delta = 0.301$, 0.206 and 0.161 for the diamond, SC and BCC lattice, respectively (see tables 1 and 3). The reason for this behaviour is the presence of the *closed loops* for the two latter lattices. They increase the number of diagrams that have to be considered in the expansion, each giving the same energy contribution as in the Néel state (for $S = \frac{1}{2}$). In other words, the quantum fluctuations become interrelated in the lattices with the closed loops and thus their contribution to the ground state energy is reduced.

The results obtained for the ground state energy reduction δ, the order parameter $\langle S_i^z \rangle$, and the nearest-neighbour correlation function $\langle S_1^z S_2^z \rangle$ for the anisotropic Heisenberg model (1) are presented in figures 2–4. The corrections to all these quantities are of the order of $\sim \gamma^2$ close to the Ising limit, with the coefficients dependent on the dimension of the lattice. By comparing the calculated energies and the correlation functions we observe that two planes coupled by an exchange interaction exhibit quantum fluctuations strongly reduced from those found for a single plane. In fact, the two-plane system is found to be somewhat closer to the 3D SC lattice than to the 2D square lattice.
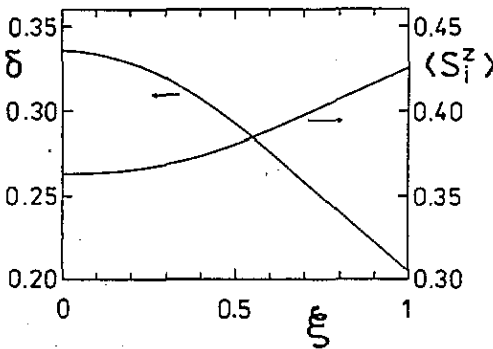
Figure 5. Quantum corrections δ to the ground state energies and the order parameter $\langle S_i^z \rangle$ in the anisotropic system described by the Heisenberg model as functions of the anisotropy ξ in the exchange interactions in a 3D lattice.
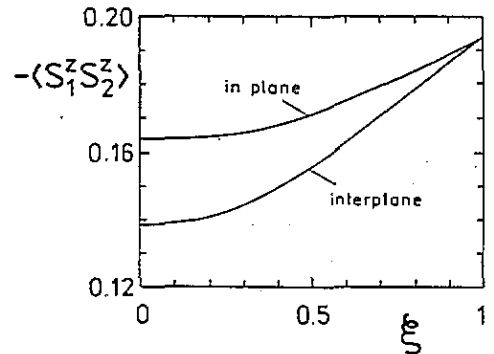
Figure 6. Spin–spin nearest-neighbour correlation functions $\langle S_1^z S_2^z \rangle$ in the anisotropic system described by the Heisenberg model as function ξ of the anisotropy in the exchange interactions in a 3D lattice.

Finally, we considered a 3D system with an anisotropic exchange interaction, as defined in equation (16). As for the cases discussed above, we have solved self-consistently equations (18) and (19) by a numerical minimization of the energy E_0 over a single variational parameter α. It has been found that a small interplane exchange interaction $J_\perp$ has almost no effect on the in plane properties, such as the energy per bond, the average magnetization $\langle S_i^z \rangle$, and the nearest-neighbour correlation function $\langle S_{ni}^z S_{nj}^z \rangle$ (see figures 5 and 6). Thus the system with $\xi = J_\perp / J_\parallel < 0.1$ remains practically equivalent to a 2D Heisenberg antiferromagnet. The quantities displayed in figures 5 and 6 start to change faster only for $\xi \simeq 0.2$ and gradually approach the limit of a 3D antiferromagnet on an SC lattice as $\xi \to 1$. The interplane correlation function $\langle S_{ni}^z S_{n+1,i}^z \rangle$ always has a lower value than that in the plane, as the independent quantum fluctuations within both planes weaken the spin order on the vertical bonds more efficiently.

4. Summary and conclusions

The results obtained in the previous section demonstrate that the variational wave function originally proposed by Bartkowski [17] is well designed for estimating the ground state energy of models of interacting spins on different lattices. It captures the essential part of the quantum fluctuations that, in the leading order, occur on the bonds between the nearest neighbours. The expansion obtained in the variational parameter converges rapidly and gives the estimated energy of the infinite 2D square lattice $E_0 = -0.3340J$ per bond, being higher only by less than 0.3% than that obtained from the Green function Monte Carlo

method, $E_0 \simeq -0.3347J$ per bond [7–9]. It is not easy to come close to this number by using analytic methods. Furthermore, the obtained energy agrees quite well with that, $E_0 = -0.3337J$, found in the projection method by Becker and co-workers [23], as well as with $E_0 = -0.3341J$ reported recently by Harris [24] for the 2D lattice and thus it may be considered to be a typical result of a local expansion around a single bond. However, the value of the magnetization obtained for the 2D square lattice, $\langle S_i^z \rangle \simeq 0.363$, is much less satisfactory. We note that the other expansions give again the values of the order parameter consistent with our result, $\langle S_i^z \rangle = 0.36$ [23], and 0.35 [24]. This points out a certain conceptual similarity of all these expansions. It demonstrates that while *local* expansions may be successfully used to describe the short-range order that determines the energy in a quantum antiferromagnet, a correct determination of the long-range order parameter (and the correlation functions at larger distance) is a much more subtle problem. It is related to the weak dependence of the energy of a quantum antiferromagnet on the actual value of $\langle S_i^z \rangle$, demonstrated by the Monte Carlo calculations for the 2D lattice [25]. While the local expansions have serious difficulties in implementing the long-range quantum fluctuations, they are correctly included in the spin wave expansion which gives the energy of $E_0 = -0.33\,499J$ and magnetization of $\langle S_i^z \rangle = 0.30686$ in a 2D square lattice [26, 27], in excellent agreement with the best Monte Carlo estimates [7–9]. Therefore, one can treat the values of $\langle S_i^z \rangle$ calculated from local expansions, including that presented here, only as qualitative information about the reduction of the long-range order parameter in various systems. It may be also concluded that quantum fluctuations that involve more distant spins play a significant role in reducing the ground state magnetization, but have only a relatively small contribution to the energy of a 2D antiferromagnet. As we have shown, their contribution is the most significant for a 1D chain, as the energy given in table 1 amounts only to 96.4% of the exact ground state energy [3].

Altogether, the expansion performed shows that *local* quantum fluctuations dominate the behaviour of the ground state of an AF Heisenberg model. The corrections to the energy and to the correlation functions are non-linear functions of the anisotropy in the exchange interactions, both for the anisotropic Heisenberg model and for the 3D antiferromagnet with weak coupling in the direction perpendicular to the planes. Thus, the Ising term dominates in the anisotropic Heisenberg model (1) with $\gamma \leqslant 0.5$, and the anisotropic antiferromagnet (16) with $\xi \leqslant 0.1$ has practically the same characteristics as a 2D system. But, of course, the presence of the exchange interaction in the third direction changes the finite-temperature properties and, in particular, influences the value of the transition temperature [28].

We would like to point out that the variational wave functions (3) and (17) used are limited to AF systems with the classical ground state consisting of two sublattices, described by the Hamiltonian with nearest-neighbour interactions. In principle, one could treat the Heisenberg systems with more extended exchange interactions in a similar way. The method cannot be applied, however, to the highly frustrated systems with an infinite range of exchange interaction, as for instance to the Kittel–Shore–Dekeyser–Lee model [29, 30] with AF exchange.

Finally, we would like to comment briefly on the result obtained for the system of two planes. It shows that the correlation functions and the ground state energy are strongly influenced by the presence of the interplane coupling. Thus, the AF ground state of the undoped $YBa_2Cu_3O_6$, where two CuO_2 planes next to each other are present, is expected to be different from that of the undoped La_2CuO_4, where the single CuO_2 planes with the frustrated interplane exchange interaction would rather behave as a 2D antiferromagnet. Indeed, these two compounds have quite different transition temperatures ($T_N \simeq 450$ K and 240 K) and the values of the order parameter ($0.65\mu_B$ and $0.55\mu_B$) [2, 31]. Our variational

calculation gives a reduction of the magnetization in a two-plane antiferromagnet of 74% of that found in a 2D square lattice, and agrees qualitatively with the reduction of 68% obtained in the spin wave theory [32]. Thus, the values of the order parameter in the undoped La_2CuO_4 and in $YBa_2Cu_3O_6$ given above may be well explained by correcting the mean field values of the respective order parameter by the respective amount of quantum fluctuations [33].

We believe that these new results on the variational wave function (3) have demonstarted the efficiency of this analytic approach for obtaining rather accurate yet simple estimates of the ground state energy in Heisenberg antiferromagnets and contributed to a better understanding of the quantum fluctuations in the systems with different lattice topology.

Acknowledgment

Appendix

Here we give more details concerning the derivation of equations (9) and (11). Let us consider first the magnetization $\langle S_0^z \rangle$, which is calculated from equation (8). The averages in the numerator and in the denominator of equation (8) contain only even powers of α, as the quantum fluctuations which occur in $|\phi_0\rangle$ have to be matched by the respective ones from $\langle \phi_0 |$. In the lowest-order one considers only one quantum fluctuation in the wave function $|\phi_0\rangle$ with respect to the Néel background, $|\psi_N\rangle$. It reverses the spin at site 0 and at one of its nearest-neighbour sites in the numerator of equation (8). The non-vanishing contribution to the average magnetization $\langle S_0^z \rangle$ is obtained if this defect is next repaired by the respective quantum fluctuation in $\langle \phi_0 |$. The denominator is expanded in the same way up to α^2 and one finds that

$$\langle S_0^z \rangle = \frac{S_0^z + z\alpha^2(S_0^z - 1)P}{1 + z\alpha^2 P}. \tag{A1}$$

This equation reproduces equation (24) given in [17].

The terms $\sim \alpha^4$ are twofold. If $S > \frac{1}{2}$, another quantum fluctuation may occur either on the same bond as the first, or at a bond which starts either at site 0, or at a neighbour of 0 with the spin reversed after the first quantum fluctuation. Next, these defects are sequentially repaired by the terms from $\langle \phi_0 |$. The second kind of contribution involves the closed loops and occurs for any value of S. It may be easily understood by considering an example of the square lattice. Two bonds that start from the site $0 \in A$ (with up spin) in x and y directions build a square, together with two other bonds that connect the neighbours of $i = 0$, labelled 1 and 2, with their common nearest neighbour, $i = 3$. Now the quantum fluctuations from $|\phi_0\rangle$ may occur, for instance, on the bonds $(0, 1)$ and $(2, 3)$. Thus, all the spins of the considered square have been flipped from the Néel configuration in the intermediate state. If we now take the terms $S_0^+ S_2^-$ and $S_3^+ S_1^-$ from the wave function $\langle \phi_0 |$, the spins of the square will be flipped back to their original positions. The resulting diagram is a closed loop on the square. Such contributions have to be counted in a combinatorial way. Thus

we define K as the number of closed loops of length four that may be constructed around any chosen bond in the lattice. It is straightforward to verify that $K = 2$, 4, and 12 for the 2D square, SC and BCC lattice, respectively. The diagrams that originate from having exactly the same quantum fluctuations on both sides of S_0^z in equation (8) are disconnected and do not contribute. Thus, taking $S = \frac{1}{2}$ one finds up to fourth order that

$$\langle S_0^z \rangle = \frac{S_0^z + z\alpha^2(S_0^z - 1)P + z\alpha^4 K(S_0^z - 1)P^3}{1 + z\alpha^2 P + z\alpha^4 K P^3}. \tag{A2}$$

Higher-order contributions occur in this case due to longer closed loops; examples of such loops were given in [19]. For topological reasons the loops always have an even number of bonds and increasing the length of the loop by two bonds results in an extra factor of $\alpha^2 P^2$ in the expansion. It is therefore straightforward to write down the general formula for $\langle S_0^z \rangle$, as given in equation (9) for $S = \frac{1}{2}$. In order to perform numerical calculations for a particular lattice up to order $2n$, one has to determine the numbers c_{2k} of closed loops of length $2k = 4, ..., 2n$ that may be constructed around a given bond.

The calculation of the ground state energy E_0, as given in equation (5), is performed in a similar way. There are two terms: the Ising part and a transverse part. Let us consider the Ising term first. In second order a single quantum fluctuation occurs either on the considered bond $(0, a)$, or on one of the outside bonds that connects site 0 (or site a) with its nearest neighbour. This quantum fluctuation has to be matched by the same term from $\langle \phi_0 |$ in order to come back to the Néel state. One finds that

$$\langle S_0^z S_a^z \rangle = \frac{1 + \alpha^2[1 - 2(z - 1)P]}{1 + \alpha^2[1 + 2(z - 1)P]}. \tag{A3}$$

In fourth order the contributions to the energy calculated for $S = \frac{1}{2}$ are twofold. First, two separate quantum fluctuations may occur: one on a bond connecting the site $i = 0$ with its nearest neighbour different from a; and another one on a bond connecting the site $i = a$ with one of its nearest neighbours different from 0. Second, a quantum fluctuation on a central bond $(0, a)$ may be accompanied by a quantum fluctuation on a parallel bond that connects the nearest neighbours of 0 and a, respectively. Such a configuration of four reversed spins on a square may be next repaired by quantum fluctuations on the other two bonds which connect the nearest neighbours (for instance, if the bond $(0, a)$ were horizontal, the compensating terms would occur on the vertical bonds). This latter term gives the lowest-order contribution due to the closed loops. We note that in both the above processes the spins 0 and a have been reversed and thus their energy contributions have the same sign as those from the Néel state. The resulting formula up to fourth order takes the form

$$\langle S_0^z S_a^z \rangle = \frac{1 + \alpha^2[1 - 2(z - 1)P] + \alpha^4(z - 1)^2 P^2 + \alpha^4 K P^2}{1 + \alpha^2[1 + 2(z - 1)P] + \alpha^4(z - 1)^2 P^2 + \alpha^4 K P^2}. \tag{A4}$$

An expansion up to higher (sixth, eighth, etc) orders is now obtained by adding the respective contributions of longer closed loops in the numerator and in the denominator.

Coming to the transverse part, $\sim (\gamma/2)(S_0^- S_a^+ + S_0^+ S_a^-)$, we note that these energy contributions contain only odd powers of α, as the term from the Hamiltonian already represents one quantum fluctuation. Thus, the lowest-order contribution is $\sim \alpha$ and occurs twice, as the quantum fluctuation on the bond $(0, a)$ may be compensated by the respective term either from $|\phi_0\rangle$ or from $\langle \phi_0 |$. In third order there is only a contribution from the closed loops of length four, of the same topology as that discussed above for $\langle S_0^z S_a^z \rangle$. By evaluating these terms one finds up to fourth order that

$$\frac{1}{2} \langle S_0^- S_a^+ + S_0^+ S_a^- \rangle = \frac{\alpha + \alpha^3 K P^2}{1 + \alpha^2[1 + 2(z - 1)P] + \alpha^4(z - 1)^2 P^2 + \alpha^4 K P^2}. \tag{A5}$$

As in the case of the Ising contribution, the higher-order terms follow from longer closed loops and can be included in the numerator of equation (A5), and in the normalization factor in the denominator. Including them in equations (A4) and (A5) results in equation (11). Bartkowski has performed a second-order expansion for the magnetization, as given in equation (A1), and an incomplete expansion up to fourth order for the energy of the form [17]

$$E_0 = -\frac{J}{4} \frac{1 + \alpha^2[1 - 2(z-1)P] + \alpha^4(z-1)^2 P^2 - 4\gamma\alpha - 4\alpha\gamma K\alpha^2 P^2}{1 + \alpha^2[1 + 2(z-1)P] + \alpha^4(z-1)^2 P^2}. \tag{A6}$$

This formula does not include the closed loop contributions in the Ising term and in the normalization factor, as given in equation (A4).

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