Independent Bond Fluctuation Approximation to the Ground State of Quantum Antiferromagnets

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A simple approach to estimation of the ground state energy of quantum antiferromagnets is developed, based on the approximation that quantum fluctuations around different bonds are independent. A transformation of the spin operators to generate bond quantum fluctuations is devised and applied to the classical ground state of the \( S = \frac{1}{2} \) Heisenberg model on the square lattice. The ground state energy estimates are as good as spin wave theory or slightly better. This simple picture of quantum fluctuations might be useful in more complex models.

The ground state energy of antiferromagnets are lowered relative to the classical energy of the Néel state by quantum effects. For the Heisenberg model, spin-wave theory\(^4\) gives a relatively good quantitative prediction of the shift. Here, I show that a simple estimation of the quantum contribution at individual bonds gives surprisingly good predictions of the ground state energy of XXZ and XY models. I also devise an explicit transformation of the spin operators that generates fluctuations around bonds when applied to the classical ground state. The energy of the resulting state is calculated on the square lattice and found to be close to the simpler estimate.

The quantum contribution to the ground state energy can mathematically be understood as arising from the Hamiltonian. The lowest energy of the diagonal part is found when the system is localized in a particular basis state, while minimizing the energy from the off-diagonal part requires a superposition of basis states. The Hamiltonian for the XXZ model is

\[
H = J \sum_{\langle i,j \rangle} [\alpha (s^x_i s^x_j + s^y_i s^y_j) + s^z_i s^z_j]
\]

\[
= J \sum_{\langle i,j \rangle} \frac{\alpha}{2} (s^+_i s^-_j + s^-_i s^+_j) + s^z_i s^z_j,
\]

where the sum runs over nearest neighbors. Here, I will only discuss values of the anisotropy parameter \( \alpha \) in the range \( 0 < \alpha \leq 1 \). The Heisenberg model is obtained with \( \alpha = 1 \). If we take as basis the states where each spin is in an eigenstate of \( s^z \), the \('zz'-\)terms in (1) are diagonal and the \('+z'-\)terms are off-diagonal.

I now restrict the further discussion to bipartite lattices, which can be divided into two sublattices with no interactions between spins on the same sublattice. The minimum energy of the diagonal terms is for antiferromagnets \( J > 0 \) found with all spins on one sublattice having \( s^z_i = +S \) (‘up’), and all spins on the other pointing the opposite way \( (s^z_i = -S) \) (‘down’), where \( S \) is the length of one spin. This is also the classical ground state. The energy is \(-JS^2\) per bond. The off-diagonal terms all have magnitude \( \alpha JS \). They couple the classical ground state to excited basis states in which one ‘up’ spin has been lowered to \( s^z_i = S - 1 \) and a neighboring ‘down’ spin has been incremented to \( s^z_j = -S + 1 \). If the number of nearest neighbors in denoted by \( Z \), each of these two spins have diagonal couplings to \( Z - 1 \) other spins of length \( S \). In the excited basis states, this diagonal energy has increased by \( 2JS(Z - 1) \). Even for \( \alpha = 1 \), this increase in diagonal energy is substantially higher than the off-diagonal coupling, so we may expect the zero-point fluctuations to be relatively small. Therefore make the approximation that quantum ground state fluctuations about different bonds are uncorrelated. To calculate the depression of ground state energy per bond we only need to take into account the basis state that the Hamiltonian of one bond couples to, with the diagonal and off-diagonal terms given above. The ground state energy per bond \( E_{XXZ} \) can then be found as the lowest eigenenergy of the matrix

\[
\begin{pmatrix}
-\alpha JS^2 & \alpha JS \\
\alpha JS & -JS^2 + 2JS(Z - 1)
\end{pmatrix}
\]

which is

\[
E_{XXZ} = -JS^2 + JS(Z - 1) - JS \sqrt{(Z - 1)^2 + \alpha^2}
\]

If we write the corresponding eigenvector in the form

\[
\begin{pmatrix}
1 \\
\eta
\end{pmatrix}
\]

the relative amplitude of the basis state with exchanged spins is then

\[
\eta = \frac{1}{\alpha} (\sqrt{(Z - 1)^2 + \alpha^2} - (Z - 1))
\]

The XY model has the Hamiltonian

\[
H_{XY} = J \sum_{\langle i,j \rangle} [s^x_i s^x_j + s^y_i s^y_j]
\]

It can easily be handled by the method developed here if it is considered the ‘XZ’ model in the chosen basis\(^2\).

\[
H_{XZ} = J \sum_{\langle i,j \rangle} [s^x_i s^x_j + s^z_i s^z_j]
\]

\[
= J \sum_{\langle i,j \rangle} \left\{ \frac{1}{4} (s^+_i s^-_j + s^-_i s^+_j + s^-_i s^-_j + s^+_i s^+_j + s^+_i s^-_j + s^-_i s^+_j) + s^z_i s^z_j \right\}
\]
The ground state and the diagonal energies are the same as for the XXZ model with \( \alpha = 0.5 \), but in addition to the \('+\rightarrow -'\) and \('-\rightarrow +'\) terms found in (11), \('+\rightarrow +'\) and \('-\rightarrow -'\) terms now appear. However, these new terms destroy the state with lowest diagonal energy so they can be disregarded for the calculation of the ground state energy by the present method. The remaining off-diagonal terms are \( JS/2 \), so the estimated ground state energy per bond becomes

\[
E_{XY} = -JS^2 + JS(Z - 1) - JS\sqrt{(Z - 1)^2 + 1/4} \tag{8}
\]

It is simple to do the calculation for other anisotropic models with antiferromagnetic spin order. Obviously, the strongest interactions should be along the z-direction. Models with interactions between i.e. \( S = \frac{1}{2} \) and \( S = 1 \) spins can also be handled by the same general method, although new expressions for both diagonal and off-diagonal terms must be devised.

Table I lists the ground state energies for the \( S = \frac{1}{2} \) Heisenberg and XY models on selected lattices, with \( J = 1 \). Shown are estimates of the values from exact methods or accurate numerical calculations (see footnotes for references), the results from first order spin wave theory \( ^5 \) and the values found by equation (11) or (8). These approximations are seen to be as good as the spin wave results, in most cases even slightly better (calculations on the square lattice XXZ model, \( \alpha < 1 \), follow below). The good agreement suggests that the simple picture of uncorrelated bond fluctuations is a reasonable representation of local correlations in the true ground state.

The energy estimates (6) and (8) do not take into account correlations between different bonds. In fact, the diagonal energy change \( 2JS(Z - 1) \) used in the derivation of (8) no longer holds when spins in a neighboring bond are exchanged. For this reason, one would expect the approximation to be best when the amplitude of spin exchange is small. Expansion of (8) to first order gives \( \eta \approx \alpha^2/2(Z - 1) \), and in fact the results in Table I are better the higher the number of nearest neighbours. For cases with \( S > \frac{1}{2} \), exchange of neighboring spins does not flip the neighboring spins completely. Hence, the relative change of the diagonal energy is smaller, and the approximation can be expected to work better for larger values of \( S \). Indeed, for the 1D \( S = 1 \) Heisenberg model, equation (8) with \( J = 1 \) gives the ground state energy \( -\sqrt{2} \sim -1.414 \), close to the very accurate numerical estimate \(-1.40 \) (the reference gives 9 more significant digits). Results in higher dimensions and/or for higher values of \( S \) are expected to be even better.

The derivation of (8) consists of taking the classical ground state and introducing uncorrelated perturbations at each bond. I call the corresponding state the Independent Bond Fluctuation (IBF) state. It is (without normalization)

\[
|IBF\rangle = \prod_{(i,j)} \left[1 - \eta s_i^- s_j^+ / 2S\right]|0\rangle \tag{9}
\]

where \( |0\rangle \) is the classical ground state and the product runs over all pairs of nearest neighbours with index \( i \) counting \('up'\)-spins and \( j \) counting \('down'\)-spins. Clearly, \( \eta \) is the amplitude of the state with spins exchanged at one bond, given by (6). This is very similar to the Local Ansatz approximation developed by Stollhoff and Fulde \( ^o \).

The relation \([s_i^+, s_j^-] = 2s_i^+\) holds generally for spin operators. In the following, the discussion is limited to the case \( S = \frac{1}{2} \), where \([s_i^+, s_j^-]|0\rangle = |0\rangle \) if spin \( i \) belongs to the sublattice pointing up. Therefore, one may treat the spin operators as bosonic with \( s_i^- \) as creation operator \( \eta s_i^- \) as destruction operator and \( s_i^+ \) as destruction operator. This is one of the ways to express the basic idea behind spin wave theory \( ^9 \). On the \('down'\)-sublattice, \( s_j^- \) destroys the classical ground state and \([s_j^-, s_j^+]|0\rangle = |0\rangle \). It might be interesting to find operators which destroy the IBF state instead, since it has an improved description of local quantum correlations in the XXZ model. \( s_j^+ \) does the job to zeroth order in \( \eta \) on the \('up'\)-sublattice, but it can be seen from (9) that terms of amplitude \(-\eta \), with a spin pointing up on one of the neighboring sites, still remain. These terms can be neutralized by adding operators that construct the same terms with amplitude \(+\eta\):

\[
s_i^+ = s_i^+ + \eta \sum_{j \in N_i} s_j^+ \tag{10}
\]

where \( N_i \) is the set of nearest neighbours to spin \( i \). This construction is not ideal, since \( s_i^+ s_i^- \) and \( s_j^- \) on neighboring sites \((i, j)\) don’t commute. A more satisfactory operator is

\[
t_i^{+(1)} = s_i^+ \pm 2\eta s_i^\pm \sum_{j \in N_i} s_j^+ \tag{11}
\]

which still destroys the IBF state to first order in \( \eta \), but also commutes with \( t_j^{-(1)} \) on neighboring sites to first order in \( \eta \). The positive sign in (11) holds on \('up'\)-sites, the negative sign on \('down'\)-sites. I now introduce the

| Model         | Reference value | Spin-wave | This work |
|---------------|-----------------|------------|-----------|
| 1D Heisenberg | -0.4431 \(^a\)  | -0.4315    | -0.4571   |
| Square Heisenberg | -0.3362 \(^b\) | -0.329     | -0.3311   |
| Cubic Heisenberg | -0.2998 \(^c\) | -0.299     | -0.2995   |
| 1D XY         | -0.318 \(^d\)   | -0.299     | -0.3090   |
| Square XY     | -0.2745 \(^e\)  | -0.27      | -0.2707   |
| Cubic XY      | -0.2640 \(^f\)  | -0.26      | -0.2625   |

\(^a\) Exact, \(^b\) Renormalisation, \(^c\) Self-consistent mean-field, \(^d\) Exact, \(^e\) Correlated basis function.
operator
\[ L = \eta \sum_{(i,j)} (s_i^- s_j^+ - s_i^+ s_j^-) \]  
(12)

where the sum runs over all pairs of nearest neighbors on the lattice, and spins of index \( i \) are on the 'up'-sublattice in \( |0\rangle \) and spins of index \( j \) are on the 'down'-sublattice. \( L \) is obviously anti-Hermitian \((L^\dagger = -L)\), so the operator transformation
\[ t_i^\pm = e^{-L} s_i^\pm e^L \]  
(13)
\[ t_j^\pm = e^{-L} s_j^\pm e^L \]  
(14)

conserves all commutation relations; the \( t \) operators obtained by this transformation are \textit{bona fide} spin-\( \frac{1}{2} \) operators, albeit delocalized on the lattice. Equation (13) can be expanded
\[ t_i^+ = s_i^+ + [L, s_i^+] + \frac{1}{24} [L, [L, s_i^+]] + \ldots \]  
(15)
\[ = s_i^+ + 2\eta s_i^z \sum_{j \in N_i} s_j^+ + \mathcal{O}(q^2) \]  
(16)

showing that \( t_i^{+(1)} \) is exactly \( t_i^+ \) expanded to first order. \( L \) can alternatively be written
\[ L = 2i\eta \sum_{(i,j)} (s_i^- s_j^+ - s_i^+ s_j^-) = 2i\eta \sum_{(i,j)} (s_i \times s_j)^z \]  
\[ = \frac{2\eta}{\alpha} [H, \sum_i s_i^- - \sum_j s_j^+] \]  
(17)

The asymmetric form of \( L \) distinguishes the transformations developed here from the Local Ansatz method\[2\], and is specific for antiferromagnetic interactions.

The \( t_i^+ \) operator destroys the \(|\text{IBF}\rangle\) state to first order, and it \textit{exactly} destroys the state \( e^{-L}|0\rangle \). This state is simply the classical ground state in the (slightly) delocalized spin operators defined by (13,14). Its' potential as a ground state candidate can be evaluated by calculating the energy per bond
\[ E^0(L) = \langle 0|e^{L}H_{\alpha}e^{-L}|0 \rangle \]  
(18)

where \((i, j)\) is any pair of nearest neighbors. I have obtained an approximate value of \( E^0(L) \) for XXZ models on the square lattice, by expanding \( e^{L}H_{\alpha}e^{-L} \) to high orders in a symbolic computation and calculating the value of terms with only \( s_\alpha \) operators (since \( \langle 0|s_i^+|0 \rangle = \langle 0|s_i^-|0 \rangle = 0 \)). In \( L \), terms were included from a part of the lattice around the \((i, j)\)-pair large enough to avoid any finite-size effects.

Table I lists the results for \( \alpha = 0.5, 0.8, 0.9 \) and 1 (in units of \( J \)). The row labelled 'Reference energy' contains low numerical estimates as described in the caption. The next row, labelled '\( E_{\text{XXZ}} \)' are calculated using formula (9). The row labelled '\( E^0(L) \), nn corr.' gives the results of expanding (13) to 7th order with the form of \( L \) given by (12) and calculating the minimum energy with \( \eta \) as a variational parameter. The values of \( \eta \) are listed below; they agree with the values found by (5) to within a few percent. To assess the convergence of the expansion, it can be noted that the biggest contribution to the energy from the 7th order term is \(-0.0002\), for \( \alpha = 1 \). Hence, the accuracy is probably sufficient for comparing the different approaches.

For all values of \( \alpha \), it is seen that \( E^0(L) \) is a poorer estimate of the ground state energy than \( E_{\text{XXZ}} \), even though the calculation of \( E_{\text{XXZ}} \) involves no free parameters. In order to improve the variational result, I have tried the calculation with further terms in the definition of \( L \). Since the expression (12) changes sign under exchange of indices \( i \) and \( j \), it is not obvious how to have terms with two spins from the same sublattice, as there is no natural way to choose the sign for a given pair. Therefore, I have only added terms between third-nearest neighbours. There are two types of 3rd nearest neighbours: one type connected by a knight’s move (two bonds in a row followed by one perpendicular bond), with parameter \( \eta_{21} \), the other connected by three bonds in row with parameter \( \eta_{30} \). Following this notation, the amplitude of terms involving nearest neighbours is called \( \eta_{10} \). For the calculation, all terms in (13) were expanded to 5th order, and 6th and 7th order terms in \( \eta_{10} \) were added. The minimum energies obtained in this fashion are listed in the row labelled '\( E^0(L) \), 3rd nn corr.' and the parameters are provided below. The lowering of the energy relative to the case with only nearest-neighbour terms is modest, just bringing the result in line with \( E_{\text{XXZ}} \) (except for \( \alpha = 1 \)). Improvements from correlations between more distant spin pairs are probably quite negligible, but lower energies might be obtained by adding 4-spin terms to \( L \).

Although the energies of states of the type \( e^{-L}|0\rangle \) are further from the true ground state energies than the simple estimate \( E_{\text{XXZ}} \) (not to mention the energies found by more elaborate methods), the existence of low-lying states of this new, simple form could still be of some interest. In particular, the concept of delocalized spin

| \( \alpha \) | 0.5 | 0.8 | 0.9 | 1.0 |
|---|---|---|---|---|
| Reference energy | -0.2706 | -0.3037 | -0.3183 | -0.3362 |
| \( E_{\text{XXZ}} \) | -0.2707 | -0.3024 | -0.3160 | -0.3311 |
| \( E^0(L) \), nn corr. | -0.2706 | -0.3018 | -0.3149 | -0.3292 |
| \( \eta \) | 0.0837 | 0.1329 | 0.1481 | 0.1629 |
| \( E^0(L) \), 3rd nn corr. | -0.2707 | -0.3024 | -0.3160 | -0.3309 |
| \( \eta_{10} \) | 0.0840 | 0.1353 | 0.1518 | 0.1670 |
| \( \eta_{21} \) | 0.0025 | 0.0092 | 0.0129 | 0.0161 |
| \( \eta_{30} \) | 0.0007 | 0.0037 | 0.0056 | 0.0073 |

**Table II.** Lowest XXZ-model energies and parameters for the state \( e^{-L}|0\rangle \) on the square lattice. Reference energies are the lowest values from the different methods listed in ref. 13, except for \( \alpha = 1 \), where the number is the same as used in Table I.
operators might be a useful tool to account for quantum effects on magnetic order in more complex contexts, where the most accurate methods are difficult to apply. The transformation (13) can also be applied to fermions, with $s^+_{\mathbf{k}}$ in (12) replaced by the creation operator $c^\dagger$ etc., and possibly used to approximate the ground state of the Hubbard model or similar models.

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[1] P. W. Anderson, Phys. Rev. 86, 694-701 (1952).
[2] G. Gomez-Santos and J. D. Joannopoulos, Phys. Rev. B. 36, 8707-8711 (1987).
[3] L. Hulthén, Arkiv Mat. Astron. Fysik 26A, 1 (1938).
[4] D. C. Mattis and C. Y. Pan, Phys. Rev. Lett. 61, 463-466 (1988).
[5] D. Chu and J.-L. Shen, Phys. Rev. B 44, R4689-R4692 (1991).
[6] E.H. Lieb and D.C. Mattis, Mathematical Physics in One Dimension (Academic Press, New York and London, 1966).
[7] D. J. J. Farnell and M. L. Ristig, cond-mat/0105386 (2001). 60, 2531-2534 (1988).
[8] S. R. White and D. A. Huse, Phys. Rev. B 48, 3844 (1993).
[9] G. Stolthoff and P. Fulde, Z Physik B 26, 257-262 (1977).
[10] T. Holstein and H. Primakoff, Phys. Rev. 58, 1098-1113 (1940).
[11] N. S. Witte, L. C. L. Hollenberg and Z. Weihong, Phys. Rev. B 55, 10412-10418 (1997).