Review

Quantum phase transitions: a variational mean-field perspective

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Abstract
To illustrate a simple mean-field-like approach for examining quantum phase transitions we consider the $J\text{-}J'$ quantum Heisenberg antiferromagnet on a square lattice. The exchange couplings $J$ and $J'$ are competing with each other. The ratio $J'/J$ is the control parameter and its change drives the transition. We adopt a variational ansatz, calculate the ground-state energy as well as the order parameter and describe the quantum phase transition inherent in the model. This description corresponds completely to the standard Landau theory of phase transitions. We also discuss how to generalize such an approach for more complicated quantum spin models.

Keywords: quantum phase transitions, square-lattice $J\text{-}J'$ Heisenberg antiferromagnet, mean-field approach

(Some figures may appear in colour only in the online journal)

1. Thermal and quantum phase transitions

Phase transitions are ubiquitous. Melting of solids, evaporation of liquids, disappearance of ferromagnetism upon heating are typical examples to name just a few.

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Thermodynamics and statistical physics provide a background for understanding phase transitions [1–3]. An important concept here is the order parameter. Its behaviour as varying some control parameter signalizes a phase transition. For the ferromagnetic–paramagnetic phase transition driven by temperature (control parameter) it is naturally to choose the total magnetization as the order parameter. The magnetization is nonzero in the low-temperature ferromagnetic phase but is zero in the high-temperature paramagnetic phase. If the order parameter vanishes (or arises) continuously with varying of the control parameter we face a continuous phase transition.

Statistical mechanics gives many exactly solvable microscopic models which exhibit phase transitions. The square-lattice Ising model first solved by Lars Onsager in 1944 [4] is probably the most famous one. Within the statistical mechanics picture, the magnetization starts to fluctuate as the temperature deviates from zero resulting in the reduction of the ground-state magnetization. As the temperature approaches the critical value, the fluctuations are extremely developed and the magnetization vanishes. Finally, it is zero for all temperatures above the critical temperature.

Interestingly, there is a similar picture for a quantum many-particle system being in the ground state (i.e., at zero temperature) where fluctuations have quantum nature. The temperature cannot serve as the control parameter. Rather, external pressure, magnetic field or competing terms in the Hamiltonian etc may be appropriate to tune the strength of quantum fluctuations, i.e., these parameters can drive the transition at zero temperature. The simplest example showing a quantum phase transition is the spin-1/2 Ising ferromagnet in a transverse magnetic field [5–7]

\[ H = J \sum_{\langle nm \rangle} \hat{s}_n^x \hat{s}_m^x - h \sum_n \hat{s}_n^z, \quad J < 0, \]  

where the first sum runs over all nearest-neighbour pairs and the second sum over all lattice sites, \( n = 1, \ldots, N \). While in the pure Ising model \( (h = 0) \) no quantum fluctuations are present, the term with the transverse field does neither commute with the Ising interaction nor with the operator of the order parameter \( \hat{S} = \sum_n \hat{s}_n^z \), thus introducing quantum fluctuations. Clearly, at zero field the ground state is the fully polarized ferromagnetic state with order parameter \( \langle \text{GS}\rangle \hat{S}\langle \text{GS} \rangle = N/2 \). Increasing the field strength the magnetization (order parameter) first remains finite (although is reduced). If the field strength approaches a critical value, the fluctuations of the order parameter become extremely developed resulting in vanishing of the magnetization. Finally, above this critical field the order parameter is zero. This picture has been confirmed experimentally [8].

Except the Ising model in the transverse field there are many other quantum spin models exhibiting quantum phase transitions. In particular, spin-1/2 Heisenberg models with competing bonds provide a large variety of models which are often appropriate to describe experimental findings in magnetic compounds [9, 10]. Below we will discuss such a quantum spin Heisenberg model in two dimensions in some detail. For this purpose we use the variational approach which is a widely used tool in theoretical physics in general [11] and in the theory of quantum many-body systems in particular [12, 13]. Typically the mean-field approximation corresponds to some replacement of operators by mean values, see, e.g., [14, 15]. In our paper we use a different approach: we consider the full quantum Hamiltonian and the mean-field idea is then implemented in a variational ansatz for the ground-state wave function.

The rest of the paper is organized as follows. First we describe the model used to study a quantum phase transition, section 2. Next, we introduce a variational ansatz and determine observables, section 3.1. The elaborated theory can be cast into the standard Landau theory of
2. The $J$–$J'$ quantum Heisenberg antiferromagnet

As already mentioned in the Introduction a canonical model to study quantum phase transitions is the spin-$1/2$ Heisenberg model with competing exchange bonds, say $J$ and $J'$,

$$
H = J \sum_{(nm)} s_n \cdot s_m + J' \sum_{(nm')} s_n \cdot s_m.
$$

(2.1)

Here the control parameter typically is the ratio of $J$ and $J'$. In what follows we call model (2.1) the $J$–$J'$ model. Let us consider a specific example for such a $J$–$J'$ model namely a square-lattice model with two different antiferromagnetic nearest-neighbour interactions $J > 0$ and $J' > 0$ as shown in figure 1. Both $J$ and $J'$ are positive, we also assume that $J' \geq J$, and the $J'$ bonds form a staggered (in contrast to, say, columnar or herringbone, see [16, 17]) covering of the square lattice.

If $J' = J$ we face the well-investigated square-lattice spin-half Heisenberg antiferromagnet, see, e.g., [18–20]. In this limit the ground state exhibits antiferromagnetic Néel-type long-range order. It is important to notice that the simple Néel product state $\Psi_{\text{Néel}} = |\uparrow\rangle |\downarrow\rangle |\uparrow\rangle |\downarrow\rangle |\uparrow\rangle |\downarrow\rangle |\uparrow\rangle |\downarrow\rangle \ldots$ (as shown pictorially on the left side of figure 2) is not an eigenstate of the quantum model. Rather, the ground state is a more complex many-body state with Néel-type long-range order, where the sublattice magnetization is reduced by quantum fluctuations to about 60% of the classical value [18–20]. Since the main features of the...
classical Néel order are present in the quantum model as well, we call this type of order semiclassical Néel order.

On the other hand, in the limit of \( J' / J \to \infty \) the ground state is of quantum nature without a classical reference state. This can be easily seen by considering an isolated spin pair coupled by the antiferromagnetic bond \( J' \): while for the Ising model (and similarly for the classical Heisenberg model) a single state \( | \uparrow \rangle | \downarrow \rangle \) (or equivalently \( | \downarrow \rangle | \uparrow \rangle \)) can serve as the ground state, for the quantum spin-1/2 Heisenberg case only the superposition of both to a spin singlet, i.e., \( ( | \uparrow \rangle | \downarrow \rangle - | \downarrow \rangle | \uparrow \rangle ) / \sqrt{2} \), is the ground state. For the lattice, at \( J'/J \to \infty \) the ground state is the regular pattern of singlets (on the bonds of strength \( J' \), as shown pictorially on the right side of figure 2), which we call valence-bond state. That is a pure quantum state with zero sublattice magnetization.

Thus, we expect that at some critical value of the ratio \( J'/J > 1 \), a phase transition between the magnetically ordered Néel phase and the valence-bond singlet phase without magnetic order occurs. Let us emphasize that for the Ising model and also for classical Heisenberg spins (i.e., \( s \) stands for the classical vector of the length \( s \)) the Néel state is the ground state for all values of antiferromagnetic \( J' \) and \( J \), and no transition takes place at all. In what follows we take the spin-1/2 \( J-J' \) model on the square lattice as a paradigm to elaborate a mean-field-like description of quantum phase transitions [21–26].

3. The variational approach: interpolating between the Néel state and the valence-bond state

3.1. Variational ansatz, the ground-state energy, and the order parameter

To interpolate between the two limiting cases, \( J'/J = 1 \) and \( J'/J \gg 1 \), we introduce the following variational state [21–26]

\[
|\Psi_{\text{var}}\rangle = \prod_{i \in A} \frac{1}{\sqrt{1 + t^2}} \left( | \uparrow \rangle_{i} | \downarrow \rangle_{i+\hat{x}} - t | \downarrow \rangle_{i} | \uparrow \rangle_{i+\hat{x}} \right).
\]  

(3.1)

The two lattice sites \( i \) and \( i + \hat{x} \) in the rhs of equation (3.1) correspond to a \( J' \) bond and thus the product is taken over all \( J' \) bonds of the lattice, see figure 1.

Furthermore, \( 0 \leq t \leq 1 \) is the variational parameter to be determined from the minimum condition for the variational energy \( E(t) = \langle \Psi_{\text{var}} | H | \Psi_{\text{var}} \rangle \). If \( t = 0 \) equation (3.1) gives the Néel state; if \( t = 1 \) equation (3.1) gives the valence-bond singlet state (i.e., the product state of the singlets on \( J' \) bonds).
After introducing the (approximate) wave function (3.1) all following calculations are more or less straightforward and no further approximations are necessary. Let us calculate the variational energy \( E(t) = \langle \Psi_{\text{var}} | H | \Psi_{\text{var}} \rangle \). We choose the numeration of sites as shown in figure 3, i.e., the sites 1 and 2 are connected by a \( J \) bond and the sites 2 and 3 are connected by a \( J' \) bond. We get

\[
(\sigma^+_1 \sigma^-_2 + \sigma^+_2 \sigma^-_1) |\Psi_{\text{var}}\rangle \\
= \ldots \frac{1}{\sqrt{1 + t^2}} (| \uparrow_1 \downarrow_2 \rangle - t | \uparrow_1 \uparrow_2 \rangle) \ldots,
\]

\[
s^+_1 s^-_2 |\Psi_{\text{var}}\rangle \\
= \ldots \left( -\frac{1}{4} \right) \frac{1}{\sqrt{1 + t^2}} (| \uparrow_1 \downarrow_2 \rangle - t | \downarrow_1 \uparrow_2 \rangle) \ldots,
\]

\[
\langle \Psi_{\text{var}} | s_1 \cdot s_2 | \Psi_{\text{var}} \rangle = -\frac{J}{1 + t^2} - \frac{1}{4} \tag{3.2}
\]

and

\[
(\sigma^+_2 \sigma^-_3 + \sigma^+_3 \sigma^-_2) |\Psi_{\text{var}}\rangle \\
= \ldots \frac{1}{\sqrt{1 + t^2}} (| \uparrow_2 \downarrow_3 \rangle - \frac{1}{\sqrt{1 + t^2}} | \downarrow_3 \uparrow_3 \rangle) \ldots \\
+ \ldots \frac{t^2}{\sqrt{1 + t^2}} (| \uparrow_1 \downarrow_2 \rangle + \frac{1}{\sqrt{1 + t^2}} | \uparrow_1 \uparrow_3 \rangle) \ldots,
\]

\[
s^+_2 s^-_3 |\Psi_{\text{var}}\rangle \\
= \ldots \left( -\frac{1}{4} \right) \frac{1}{\sqrt{1 + t^2}} (| \uparrow_1 \downarrow_2 \rangle + t | \downarrow_1 \uparrow_2 \rangle) \\
\times \frac{1}{\sqrt{1 + t^2}} (| \downarrow_3 \downarrow_3 \rangle + t | \downarrow_3 \uparrow_3 \rangle) \ldots,
\]

\[
\langle \Psi_{\text{var}} | s_2 \cdot s_1 | \Psi_{\text{var}} \rangle = -\frac{1}{4} \left( \frac{1 - t^2}{1 + t^2} \right)^2. \tag{3.3}
\]

Combining equations (3.2) and (3.3) we find

\[
\frac{E(t)}{N} = \frac{\langle \Psi_{\text{var}} | H | \Psi_{\text{var}} \rangle}{N} \\
= -\frac{J'}{2} \frac{t}{1 + t^2} - \frac{J'}{8} - (z - 1)J \left( \frac{1 - t^2}{1 + t^2} \right)^2,
\tag{3.4}
\]

where \( z \) is the number of nearest neighbours, i.e., \( z = 4 \) for the square lattice.

Next task is to find the value of \( t \) which yields the minimum of \( E(t) \). Since

\[
\frac{d}{dt} \frac{E(t)}{N} = \frac{J't^4 - 6Jt^3 + 6J - J'}{2(1 + t^2)^3}, \tag{3.5}
\]

we get a fourth order algebraic equation with respect to \( t \):

\[
J't^4 - 6Jt^3 + 6J - J' = (J't^2 - 6J + J')(t^2 - 1) = 0. \tag{3.6}
\]
Equation (3.6) has the following solutions:

\[ t_1 = -1, \]
\[ t_2 = \frac{3J}{J'} - \sqrt{\frac{(3J)^2}{J'} - 1}, \]
\[ t_3 = 1, \]
\[ t_4 = \frac{3J}{J'} + \sqrt{\frac{(3J)^2}{J'} - 1}. \]  

The solutions \( t_1 \) and \( t_3 \) exist for all \( J' \), whereas the solutions \( t_2 \) and \( t_4 \) are real for \( J' \leq 3J \) only. However, we have to discard the solutions \( t_1 \) and \( t_4 \), because they do not obey the imposed restriction \( 0 \leq t \leq 1 \). Now, \( E(t)/N \) is minimal for

\[ t = \begin{cases} 
\frac{3J}{J'} - \sqrt{\frac{(3J)^2}{J'} - 1}, & J' \leq 3J, \\
1, & J' > 3J.
\end{cases} \]  

Thus, the ground-state energy (per site) is given by

\[ \frac{E_0}{N} = \begin{cases} 
-\frac{3J'}{8} - \frac{3J}{8} \left(1 - \frac{J'}{3J}\right)^2, & J' \leq 3J, \\
-\frac{3J'}{8}, & J' > 3J.
\end{cases} \]  

Following Ehrenfest’s classification of phase transitions [1], we may inspect the derivatives of the ground-state energy (that plays here the role of the relevant thermodynamic potential) with respect to the control parameter \( J' \). Easily we find that \( \partial E_0/\partial J' \) is continuous everywhere, but the second derivative, \( \partial^2 E_0/\partial J'^2 \), has a jump at \( J' = 3J \), see figure 4. Therefore, we have a first indication that there is a continuous quantum phase transition driven by \( J'/J \).
To confirm this finding, we calculate the variational sublattice magnetization (per site) \( m(t) = \langle \Psi_{\text{var}} | s^z_1 | \Psi_{\text{var}} \rangle \), that will yield the relevant order parameter. Since
\[
\langle s^z_1 | \Psi_{\text{var}} \rangle = \frac{1}{2} \frac{1}{\sqrt{1 + t^2}} (\langle \uparrow \downarrow \rangle + t \langle \downarrow \uparrow \rangle) \ldots,
\]
we arrive at
\[
m(t) = \frac{1}{2} \left( 1 - \frac{t^2}{1 + t^2} \right)
\]
for the variational magnetization at a site on the sublattice \( A \). For the corresponding magnetization at a site on the sublattice \( B \) the same expression, but with the opposite sign, is valid. Inserting the optimal \( t \) from equation (3.8) and (for \( J' \leq 3J \)) using
\[
2m_0 = (1 - r^2 + r\sqrt{r^2 - 1})/(r^2 - r\sqrt{r^2 - 1}) = \sqrt{r^2 - 1}/r, \quad r \equiv 3J/J',
\]
we get for the order parameter
\[
m_0 = \begin{cases} 
\frac{1}{2} \sqrt{1 + J'/J} \left( 1 - \frac{J'}{3J} \right), & J' \leq 3J, \\
0, & J' > 3J.
\end{cases}
\]
In accordance with the findings for the ground-state energy, equation (3.12) yields a continuous transition with a quantum critical point at \( J' = 3J \) and a critical exponent \( \beta = 1/2 \) obvious from the behaviour of \( m_0 \) as \( J' \to J' - 0 \). Moreover, we have \( m_0 = \sqrt{2}/3 \approx 0.471 \) at \( J' = J \), i.e., already within our simple approach the sublattice magnetization is reduced by quantum fluctuations compared to its classical value \( m_0^{\text{class}} = 1/2 \). Knowing the variational wave function (3.1) with the variational parameter given in equation (3.8) we are able to calculate any observable quantity.

As reported above the critical index of the order parameter is that of a mean-field theory. The question arises how the mean-field character of our approach is evident. The crucial point is the product form of our wave function (3.1), i.e., there is no mutual correlation between the individual species of the system (i.e., the dimers on the \( J' \) bonds) in our wave function.

3.2. Landau theory

Due to the mean-field character of our approach it is natural to ask whether the famous Landau theory \([1, 27]\) is applicable to describe the critical behaviour discussed above. Indeed, our approach can be cast into the standard Landau theory of phase transitions. The starting point of the Landau theory is the expansion of the (variational) free energy as a function of the order parameter. Then the free energy should be minimized with respect to the order parameter. In our case, we need an expansion of the ground-state energy in powers of the sublattice magnetization. To get such an expansion, we use equation (3.11) to express \( t \) in terms of \( m \), that is, \( t(m) = \sqrt{(1 - 2m)/(1 + 2m)} \). We substitute \( t(m) \) into equation (3.4) and get
\[
\frac{E(m)}{N} = -\frac{J'}{4} \sqrt{1 - 4m^2} - \frac{J'}{8} - \frac{3}{2} Jm^2.
\]
Then expanding \( E(m)/N \) (3.13) in powers of \( m \) yields
\[
\frac{E(m)}{N} = -\frac{3}{8} J' + \frac{1}{2} (J' - 3J)m^2 + \frac{1}{2} Jm^4 + \cdots.
\]
This is the variational ground-state energy (per site) as a function of the (small) order parameter \( m \).

Within Landau’s theory of thermal phase transitions [1, 27], the simplest (i.e., the case of a scalar order parameter \( m \)) starting point is the following (variational) free energy expansion:

\[
F (T, m) = F (T, m = 0) + A(T)m^2 + Bm^4, \\
A(T) = a(T - T_c), \quad a > 0, \quad B > 0.
\]  

(3.15)

At the critical temperature \( T = T_c \), the coefficient \( A(T) \) changes its sign resulting in a qualitative change of the dependence \( F(T, m) \). The order parameter \( m \) must realize the minimum of \( F(T, m) \) and therefore it has the following temperature dependence:

\[
m_0(T) \propto \begin{cases} 
\sqrt{T_c - T}, & T \leq T_c, \\
0, & T > T_c.
\end{cases}
\]  

(3.16)

Thus, the critical exponent \( \beta = 1/2 \).

Clearly, equation (3.14) is a counterpart of equation (3.15). In the upper and middle panels of figure 5 we illustrate the qualitative change of the dependence \( E(m) \), see equations (3.13), (3.14), as the control parameter \( J'/J \) crosses the critical value \( J_c'/J = 3 \). Furthermore, in the lower panel of figure 5 we illustrate the dependence of \( m_0 \) on \( J'/J \),

\[
m_0 = \begin{cases} 
\sqrt[3]{J - J'/2}, & J' \leq 3J, \\
0, & J' > 3J,
\end{cases}
\]  

(3.17)

as the control parameter \( J'/J \) crosses the critical value \( J_c'/J = 3 \). Note that equation (3.17) corresponds to equation (3.16), and, moreover, it agrees with equation (3.12): the latter equation transforms into the former one if we assume that \( J' \to 3J - 0 \). Really, for \( J' \approx 3J - 0 \)

\[
m_0 \approx \frac{1}{2} \sqrt{2 \left( 1 - \frac{J'}{3J} \right)} = \sqrt[3]{\frac{3J - J'}{6J}} \approx \sqrt[3]{\frac{3J - J'}{2J'}}.
\]

Exploiting the relation of our approach to the Landau theory we can go one step forward and consider now the effects of the spatial variation of the order parameter within Landau–Ginzburg theory. The spatially dependent free-energy density now contains besides the local term attached to \( J' \)-bonds corresponding to (3.15) (however, with a space-dependent \( m \)) also the non-local gradient term stemmed from \( J \)-bonds that is proportional to \( |\nabla m|^2 \).

Hence, we allow the variational parameter \( t \) in equation (3.1) to be spatially dependent. Equivalently, we may assume the variational sublattice magnetization (per site) \( m \) to be space dependent since both quantities are tied together by equation (3.11). After relaxing the condition of uniform \( m \), we have to reconsider equation (3.13) for the variational ground-state energy \( E(m) \) which becomes now a functional of \( m(r) \). Recalling its derivation we conclude that now

\[
\frac{E [m(r)]}{N} = - \frac{J'}{4N} \sum_r \left( \sqrt{1 - 4m^2(r)} + \frac{1}{2} \right) - \frac{J}{2N} \\
\times \sum_r m(r)(m(r + q_i) + m(r + q_1 + q_3) + m(r + q_2)).
\]  

(3.18)

Here \( r \) runs over \( N = N/2 \) sites of the square lattice defined by, say, the left sites of the dimer bonds, see figure 6. It is convenient to rearrange the terms in the second sum in equation (3.18) replacing \( m(r)m(r + q_i) \) by \( (m(r - q_i)m(r) + m(r)m(r + q_i))/2 \) and so
Figure 5. Upper panel: the variational ground-state energy $E/N$ versus $m$ at different values of the control parameter $J'/J$. Thin dashed lines correspond to equation (3.14) (small $m$ approximation) and thick solid lines correspond to equation (3.13) (full expression for arbitrary $m$). Middle panel: $(E(m) - E(0))/N$ versus $m$ for the same values of the control parameter as in the upper panel. Lower panel: the order parameter $m_0$ as a function of the control parameter $J'/J$. The thin dashed line corresponds to equation (3.17) (small $m$ approximation) and the thick solid line corresponds to equation (3.12) (full expression for arbitrary $m$).
on. We assume \( m \) to be a slowly varying function. Therefore we can expand
\[
m(r + q_1) \approx m(r) + q_1 \cdot \nabla m(r) + q_1 \cdot \nabla(m(r))/2
\]
and so on. Furthermore, we may replace the sum by the integral:
\[
\int_V dV \left( 1/N \sum_r \cdots \right) \rightarrow \int_V dV \cdots
\]
where \( V = (\sqrt{2}a)^2N \) and \( a \) is the edge length of the square-lattice cell in figure 1. While in the first term in the rhs in equation (3.18) we have simply to expand the square root in powers of \( m \), in the second term we have to integrate by parts, neglect the boundary terms, insert \( q_1 = \sqrt{2}a(1, 0) \), and take into account that
\[
\nabla = \nabla_{rr} \quad (\partial_{x_x} \partial_{x_y}).
\]
Finally, we arrive at the following result:
\[
\frac{E[m(r)]}{N} = \frac{1}{V} \int_V dV e(m(r)),
\]
\[
e(m(r)) = -\frac{3J'}{8} + \frac{J' - 3J}{2} m^2(r) + \frac{J'}{2} m^4(r)
\]
\[
+ \frac{3a^2J'}{2} |\nabla m(r)|^2,
\]
i.e., at a field theory. It should be underlined that equation (3.19) does not represent the true field theory of the model (2.1), see section 3.3, since it is restricted only to the imposed variational states given in equation (3.1).

Landau–Ginzburg theory, when the term with the fourth power is neglected, allows to obtain the correlation function \( \langle m(r_1)m(r_2) \rangle \). It decays exponentially, \( \propto \exp(-|r_1 - r_2|/\xi) \), with the correlation length \( \xi \). The correlation length diverges at the critical point \( J'_c = 3J \) with the exponent \( \nu = 1/2 \), i.e., \( \xi \propto 1/\sqrt{|J' - J'_c|} \).

3.3. Beyond the mean-field treatment

The model discussed above at the mean-field level has been studied using more sophisticated approaches. In particular, the conjecture that the quantum phase transition present in the model may belong to a new universality class [16] has stimulated further studies of the model [17]. Let us explain this issue in more detail.

Wenzel, Bogacz, and Janke studied the spin-1/2 \( J-J' \) square-lattice Heisenberg antiferromagnet with the staggered arrangement of \( J' \) bonds (i.e., the \( J' \)-bond pattern as in figure 1) by means of (stochastic series expansion) quantum Monte Carlo simulations [16]. To probe the nature of the quantum phase transition, they calculated several well-known observables such as the staggered magnetization, the correlation length, and the spin stiffness. All observables indicate a single phase transition and the critical point is determined as...
Note that the critical point, $J_c/J = 3.5196(2)$. Note that the critical point, $J_c/J = 3$, obtained by our simple variational ansatz (3.1), is in reasonable agreement with this number. However, in contrast to a general belief, they found that the critical exponent $\nu$ obtained by analysing the data for all observables according to a finite-size scaling ansatz is $\nu = 0.689(5)$. This quantity is smaller than the standard three-dimensional classical Heisenberg model (i.e., $O(3)$) universality class $\nu = 0.7112(5)$. This contradicts a common wisdom: quantum phase transition can be mapped onto classical phase transition in one higher dimension and, in general, one expects that the quantum phase transition in $D$ space dimensions is in the universality class of the $(D + 1)$-dimensional classical model [5, 16, 17]. In the second paper [16], Wenzel and Janke extended their studies for more geometric arrangements of competing $J'$ bonds and confirmed that the critical exponent $\nu$ for other considered coupled-dimer magnets is in excellent agreement with the classical $O(3)$ universality class.

A resolution to this puzzle put forward by the numerics of [16] was proposed by L Fritz et al [17]. They showed that there are indeed two different classes of coupled-dimer magnets. While the first class (consisting, in particular, of the columnar-dimer [16] or bilayer square-lattice systems) follows the standard $O(3)$ universality class, the low-energy quantum field theory of the other class (consisting, in particular, of the staggered-dimer [16] or herringbone-dimer square-lattice systems) is characterized by an additional cubic interaction of critical fluctuations, which has no classical analogue. As a result, the asymptotic critical exponents are of the $O(3)$ universality class, but anomalously large corrections to scaling arise from this cubic interaction term. The authors of [17] also presented quantum Monte Carlo simulations that can be consistently interpreted in terms of critical exponents of the standard $O(3)$ universality class, but with anomalously large corrections to scaling.

Clearly, the discussion of [16, 17] which is based on such refined techniques as quantum Monte Carlo, effective low-energy quantum field theory and renormalization-group analysis etc is unreachable at the mean-field level. The mean-field approach based on equation (3.1) cannot differ between the two different classes of coupled-dimer magnets. In general, the shortcomings of the mean-field theories were discussed in many papers in the past. We do not want to repeat these discussions and refer an interested reader to, e.g., a recent review by Strečka and Jaščur [28].

4. Generalizations

Our variational approach allows a straightforward discussion of modifications of the $J\sim J'$ model considered above in some detail. In particular, we may modify the model in such a way that we can influence the strength of quantum fluctuations, e.g., by anisotropy, by increasing the spin quantum number $s$, or by adding frustrating next-nearest-neighbour interactions. In what follows we will present a brief discussion of such modifications.

4.1. The easy-axis XXZ $J\sim J'$ model

First we consider the anisotropic XXZ model (instead of the isotropic XXX Heisenberg model in equation (2.1)) [25]. Introducing easy-axis anisotropy permits to diminish the quantum fluctuations by increasing the amount of the Ising interaction. We consider the Hamiltonian
\[
H = J \sum_{(mm)} (s_x^m s_x^m + s_y^m s_y^m + \Delta s_z^m s_z^m) + J' \sum_{(mm)'} (s_x^m s_x^m + s_y^m s_y^m + \Delta s_z^m s_z^m)
\]

(4.1)

with \( \Delta \geq 1 \). At \( \Delta = 1 \) the model (4.1) coincides with equation (2.1), and in the limit \( \Delta \to \infty \) it yields the Ising model, i.e., a model without quantum fluctuations. Using the variational state given in equation (3.1) and performing corresponding calculations along the lines illustrated in section 3 we arrive at

\[
\frac{E(t)}{N} = -\frac{J'}{2} t \left[ \frac{\Delta}{2} \right] + \Delta \left[ 1 - \frac{1}{2} \left( \frac{1}{1 + \Delta^2} \right) \right] - \frac{3 \Delta J}{8} \left( \frac{1 - t^2}{1 + t^2} \right)^2,
\]

(4.2)

see equation (3.4). The variational energy (4.2) is minimal for

\[
t = \begin{cases} 
\frac{3 \Delta J}{J'} & \text{if } J' \leq 3 \Delta J, \\
1 & \text{if } J' > 3 \Delta J,
\end{cases}
\]

(4.3)

see equation (3.8), and the ground-state energy (per site) is given by

\[
\frac{E_0}{N} = \begin{cases} 
\frac{(2 + \Delta J')}{8} \left( 1 - \frac{J'}{3 \Delta J} \right)^2 & \text{if } J' \leq 3 \Delta J, \\
\frac{(2 + \Delta J')}{8} & \text{if } J' > 3 \Delta J,
\end{cases}
\]

(4.4)

see equation (3.9). For the order parameter, instead of equation (3.12), we have

\[
m_0 = \begin{cases} 
\frac{1}{2} \sqrt{\left( 1 + \frac{J'}{3 \Delta J} \right) \left( 1 - \frac{J'}{3 \Delta J} \right)} & \text{if } J' \leq 3 \Delta J, \\
0 & \text{if } J' > 3 \Delta J.
\end{cases}
\]

(4.5)

Finally, the Landau-like variational ground-state energy (per site) becomes

\[
\frac{E(m)}{N} = \frac{2 + \Delta J'}{8} t^2 + \frac{1}{2} (J' - 3 \Delta J) m^2 + \frac{1}{2} J' m^4 + \cdots
\]

(4.6)

see equation (3.14).

As can be seen from the reported formulas (4.4), (4.5), and (4.6), the quantum phase transition point \( J' \) is proportional to \( \Delta \), i.e., \( J'/J \) tends to infinity in the Ising limit \( \Delta \to \infty \). With increase of the Ising anisotropy \( \Delta \) the quantum fluctuations are reduced, thus pushing \( J' \) to higher values. In the pure Ising limit the only remaining terms in the Hamiltonian (4.1) are the Ising interactions and the quantum critical point for transition into singlet-product state disappears; \( J'/J \to \infty \). In other words, in the pure Ising limit the ground state is of the Néel type for all \( J'/J \). For further details see [25].

4.2. The J–J’ model for higher spin quantum numbers \( s > 1/2 \)

Another classical limit occurs when the spin value increases. Let us discuss briefly how to treat higher spin quantum numbers \( s = 1, 3/2, 2, \ldots \). For simplicity, we consider here the case \( s = 1 \) only and refer the interested reader to [26], where the cases \( s = 1, s = 3/2, \) and \( s = 2 \) are discussed. For \( s = 1 \), at each site one has three possible spin states: \( |1, 1 \rangle \equiv | \uparrow \rangle \).
If $J' = J$ we again have semiclassical two-sublattice Néel-type order where all spins, say, on the sublattice $A$ tend to be in the spin-up state $|\uparrow\rangle$, and all spins on the sublattice $B$ are preferably in the spin-down state $|\downarrow\rangle$. If $J' \gg J$ we again expect the singlet state on the $J'$ bonds. However, now the singlet state is composed of two spins with $s = 1$. One can easily find the singlet eigenstate in the subspace with $S^z = 0$, i.e., among the eigenstates like $a|\uparrow\downarrow\rangle + b|00\rangle + c|\downarrow\downarrow\rangle$, where the coefficients $a$, $b$, and $c$ are to be found. Using the relations $s^z|\uparrow\rangle = 0$, $s^z|0\rangle = \sqrt{2}|\downarrow\rangle$, and $s^z|\downarrow\rangle = 0$, one finds the following three eigenstates of the operator $\mathbf{s}_1 \cdot \mathbf{s}_2$: $|\uparrow\downarrow\rangle - |00\rangle + |\downarrow\downarrow\rangle$ (singlet) with the energy $-2$, $-|\uparrow\downarrow\rangle + 2|\downarrow\downarrow\rangle$ (triplet) with the energy $-1$, and $|\uparrow\downarrow\rangle + |00\rangle + |\downarrow\downarrow\rangle$ (quintuplet) with the energy $1$.

Bearing this in mind, we modify accordingly the variational state in equation (3.1) and assume

$$
|\Psi_{\text{var}}\rangle = \prod_{i \in A} \frac{1}{\sqrt{1 + t_1^2 + t_2^2}} \times (|\uparrow\downarrow\rangle - t_1|00\rangle + t_2|\downarrow\downarrow\rangle),
$$

(4.7)

where $t_1$ and $t_2$ are the variational parameters. For $t_1 = t_2 = 0$ equation (4.7) reproduces the Néel state and for $t_1 = t_2 = 1$ it gives the singlet-product state. The variational ground-state energy (per site) and the variational sublattice magnetization (per site) are calculated as

$$
\frac{E(t_1, t_2)}{N} = \frac{\langle \Psi_{\text{var}} | H | \Psi_{\text{var}} \rangle}{N} = -\frac{J' + 2t_1^2}{2} - \frac{3J}{2} \left( \frac{1 - t_1^2}{1 + t_1^2 + t_2^2} \right)^2
$$

(4.8)

and

$$
m(t_1, t_2) = \langle \Psi_{\text{var}} | s_i^z | \Psi_{\text{var}} \rangle = \frac{1 - t_2^2}{1 + t_1^2 + t_2^2}.
$$

(4.9)

Now we have to minimize $E(t_1, t_2)/N$ (4.8) with respect to two variational parameters, $t_1$ and $t_2$. We obtain a set of two coupled equations for $t_1$ and $t_2$ which can be solved numerically. Numerics yield $J'/J = 8$ and $\beta = 1/2$. By inspecting the critical value $J'/J$ for $s = 1/2, 1, 3/2, 2$ in [26] the relation

$$
J'/J = 4s(s + 1)
$$

(4.10)

was found. This scaling law for $J'$ (as $s(s + 1)$) has been confirmed by other methods such as the coupled cluster method [26] or the bond-operator approach [29]. As can be seen from equation (4.10), in the classical limit $s \to \infty$ the quantum phase transition to the singlet-product state disappears: $J'/J \to 0$ and the Néel state persists for any finite $J'$.

4.3. $J' = J_2$ model

A further extension of the basic model (2.1) is given by introducing a frustrating antiferromagnetic next-nearest-neighbour interaction $J_2$. Note that in the presence of frustration the powerful quantum Monte Carlo method used for the basic (unfrustrated) model (2.1), see [16, 17], is not applicable because of the sign problem [30].
The Hamiltonian of the $J-J'-J_2$ model reads
\[
H = J \sum_{\langle nm \rangle} s_n \cdot s_m + J' \sum_{\langle\langle nm \rangle\rangle} s_n \cdot s_m
+ J_2 \sum_{\langle\langle nm \rangle\rangle} s_n \cdot s_m,
\] (4.11)
where the third sum in the rhs of equation (4.11) runs over all next-nearest-neighbour bonds with the strength $J_2 \geq 0$, see figure 7. Now, in addition to calculations (3.2) and (3.3), we have to find
\[
\langle s_1^+ s_3^- + s_1^+ s_3^- \rangle |\psi_{\text{var}}\rangle
\]
\[
= \ldots (-t) \frac{1}{\sqrt{1 + t^2}} |\uparrow_1 \uparrow_2 \rangle \frac{1}{\sqrt{1 + t^2}} |\downarrow_3 \downarrow_{3+\hat{z}} \rangle \ldots
\]
\[
+ \ldots (-t) \frac{1}{\sqrt{1 + t^2}} |\downarrow_1 \downarrow_2 \rangle \frac{1}{\sqrt{1 + t^2}} |\uparrow_3 \uparrow_{3+\hat{z}} \rangle \ldots,
\]
\[
s_1^+ s_3^- |\psi_{\text{var}}\rangle
\]
\[
= \ldots \left( + \frac{1}{4} \right) \frac{1}{\sqrt{1 + t^2}} \langle |\uparrow_1 \uparrow_2 \rangle + t |\downarrow_1 \downarrow_2 \rangle \rangle
\]
\[
\times \frac{1}{\sqrt{1 + t^2}} \langle |\uparrow_3 \downarrow_{3+\hat{z}} \rangle + t |\downarrow_3 \uparrow_{3+\hat{z}} \rangle \rangle \ldots,
\]
\[
\langle \psi_{\text{var}} | s_1 \cdot s_3 | \psi_{\text{var}} \rangle = + \frac{1}{4} \left( \frac{1 - t^2}{1 + t^2} \right)^2,
\] (4.12)
see figure 7. Importantly, the sign of $\langle \psi_{\text{var}} | s_1 \cdot s_3 | \psi_{\text{var}} \rangle$, see equation (4.12), is opposite to the sign of $\langle \psi_{\text{var}} | s_2 \cdot s_3 | \psi_{\text{var}} \rangle$, see equation (3.3). Summing the contributions of all bonds, i.e., of $N/2$ $J'$ bonds, $3N/2$ $J$ bonds, and $2N$ $J_2$ bonds, we arrive at
\[
E(t) \equiv \frac{\langle \psi_{\text{var}} | H | \psi_{\text{var}} \rangle}{N}
\]
\[
= - \frac{J'}{2} \frac{t}{1 + t^2} - \frac{J'}{8} \frac{3(1 - t^2)^2}{1 + t^2}
\]
\[
+ \frac{J_2}{2} \frac{(1 - t^2)^2}{1 + t^2},
\] (4.13)
see equation (3.4). Clearly, the last two terms in equation (4.13) can be combined and after introducing the effective interaction

\[ J_{\text{eff}} = J - \frac{4}{3}J_2 \]  

(4.14)
equation (4.13) becomes identical to equation (3.4) with \( J_{\text{eff}} \) (4.14) instead of \( J \). For the critical point we get \( J' = 3J_{\text{eff}} = 3J - 4J_2 \). Clearly, the frustrating coupling \( J_2 \) suppresses \( J' \) and acts in favour of the magnetically disordered singlet-product state.

We may also consider the special limit of identical nearest-neighbour bonds, i.e., \( J' = J \). By renaming \( J' = J = J_1 \) we end up at the celebrated \( J_1-J_2 \) model on the square lattice. Our approach yields for the critical value of \( J_2 \), where the Néel order gives way for the valence-bond state, \( J_2^{\text{cr}}/J_1 = 1/2 \). This value is not far from \( J_2^{\text{cr}}/J_1 = 0.4 \ldots 0.45 \) obtained by more sophisticated methods for the critical frustration where the Néel order breaks down in the \( J_1-J_2 \) model [20, 31, 32]. Moreover, recent calculations using density matrix renormalization group approach with explicit implementation of SU(2) spin rotation symmetry in [32] have found a gapless spin-liquid state for \( 0.44 < J_2/J_1 < 0.5 \) and the transition to a gapped valence-bond phase takes place only at \( J_2/J_1 = 0.5 \).

The order parameter \( m_0 \) (sublattice magnetization per site) as a function of \( J_2 \) can be easily calculated by substituting \( J'/J = J_1/(J_1 - 4J_2/3) \) in equation (3.12). We show this dependence of \( m_0 \) on \( J_2 \) in figure 8.

4.4. The \( J-J' \) model on other lattices

The elaborated approach to examine quantum phase transitions in quantum Heisenberg antiferromagnets with competing bonds can be straightforwardly applied to other lattices. In case of unfrustrated lattices, e.g., the bilayer square-lattice [22], for the isotropic \( s = 1/2 \) model the calculations presented in section 3 are still valid. However, the number of nearest neighbours \( z \) is a relevant parameter, cf equation (3.4), and \( z \) has to be taken for the lattice under consideration. Thus, for the critical value we then have \( J_2' = (z-1)J \). Another example is the so-called CaVO (or 1/5-depleted square) lattice which is used to describe the magnetic properties of CaV_4O_9 [21, 33, 34]. For this lattice \( z = 3 \) and therefore \( J_2' = 2J \) that is in a reasonable agreement with quantum Monte Carlo data \( J_2'/J \approx 1.65 \) [35, 36].

Figure 8. The order parameter \( m_0 \) for the \( J_1-J_2 \) model (i.e., at \( J = J' = J_1 \)) calculated within the mean-field approach (3.1). The Néel order breaks down at \( J_2^{\text{cr}}/J_1 = 1/2 \).
A more interesting situation can appear on non-bipartite lattices, where due to geometrical frustrations the semiclassical magnetic order typically is non-collinear. As an example, we consider the star lattice, see figure 9. This more exotic lattice is one of the 11 uniform Archimedean tilings in dimension $D = 2$ [21, 33, 34]. The Hamiltonian of the model is given
in equation (2.1), however, now the first sum runs over all triangular bonds and the second one over all dimer bonds, see figure 9. For the uniform lattice both bonds, the triangular and dimer ones, have the same strength. In this case, two variants of a semiclassical ground state were discussed (analogues of the Néel state for the square lattice): (i) the so-called $\sqrt{3} \times \sqrt{3}$ state and (ii) the so-called $\mathbf{q} = 0$ state, see the two upper panels in figure 10. These states should appear in equation (3.1) instead of the Néel state.

The calculations for the star-lattice model can be sketched as follows. We consider either the $\sqrt{3} \times \sqrt{3}$ state or the $\mathbf{q} = 0$ state, see figure 10. Since $\mathbf{s}_n \cdot \mathbf{s}_m$ is rotationally invariant in the spin space, we may choose the $z$ axis in the spin space within the plane defined by the $\sqrt{3} \times \sqrt{3}$ or $\mathbf{q} = 0$ state (both are coplanar states). Then, we rotate the spins around the $y$ axis by an angle $\alpha$ which is site dependent, i.e., we perform local rotations

$$
\begin{align*}
\mathbf{s}^x &\rightarrow \tilde{\mathbf{s}}^x = \cos \alpha \, \mathbf{s}^x - \sin \alpha \, \mathbf{s}^z, \\
\mathbf{s}^y &\rightarrow \tilde{\mathbf{s}}^y = \mathbf{s}^y, \\
\mathbf{s}^z &\rightarrow \tilde{\mathbf{s}}^z = \sin \alpha \, \mathbf{s}^x + \cos \alpha \, \mathbf{s}^z
\end{align*}
$$

(4.15)

with $\alpha = \pi$ for ‘magenta’ sites, $\alpha = -\pi/3$ for ‘green’ sites, and $\alpha = \pi/3$ for ‘cyan’ sites, see figure 10. Clearly, the spin state at all sites shown in the two upper panels of figure 10 is now the eigenstate of the operator $\tilde{\delta}^z$ (in the rotated coordinate frame) with the eigenvalues $+1/2$ (dark sites) or $-1/2$ (light sites). We denote them $| \uparrow \uparrow \rangle$ and $| \downarrow \downarrow \rangle$, respectively. Note, however, that in the rotated coordinates the Hamiltonian becomes more complicated, since

$$
\begin{align*}
\mathbf{s}_n \cdot \mathbf{s}_m = \cos (\alpha_n - \alpha_m) &\left( \tilde{\mathbf{s}}_n^x \tilde{\mathbf{s}}_m^x + \tilde{\mathbf{s}}_n^z \tilde{\mathbf{s}}_m^z \right) \\
&+ \tilde{\mathbf{s}}_n^y \tilde{\mathbf{s}}_m^y - \sin (\alpha_n - \alpha_m) \left( \tilde{\mathbf{s}}_n^x \tilde{\mathbf{s}}_m^z - \tilde{\mathbf{s}}_n^z \tilde{\mathbf{s}}_m^x \right).
\end{align*}
$$

(4.16)

Now we adopt a variational state rewriting equation (3.1) in the form:

$$
| \Psi_{\text{var}} \rangle = \prod_{(nm)} \frac{1}{\sqrt{1 + t^2}} \left( | \uparrow_n \downarrow_m \rangle - t | \downarrow_n \uparrow_m \rangle \right),
$$

(4.17)

where the product runs over all dimer bonds $J'$ of the star lattice. Next, we have to calculate the contribution to the variational energy from different bonds. In total there are $3N/2$ bonds: $N/2$ of them are dimer bonds and $N$ of them are triangular bonds. The contribution of the dimer bonds is given by equation (3.2). The contribution of the triangular bond is given by equation (3.3) with taking into account the factor $1/2$ stemming from $\cos(\alpha_n - \alpha_m) = 1/2$ in equation (4.16). As a result, we obtain for the variational energy $E(t)$ the following formula:

$$
\frac{E(t)}{N} = \frac{J'}{2} \left( \frac{t}{1 + t^2} + \frac{1}{4} \right) - \frac{J}{8} \left( \frac{1 - t}{1 + t^2} \right)^2,
$$

(4.18)

see equation (3.4). The obtained variational energy implies $J_c = J$: one arrives at this outcome simply by comparing equation (4.18) and equation (3.4). Thus for the uniform lattice the magnetic order is already unstable, and, therefore, this result may serve as an indication of the absence of magnetic order for the star-lattice spin-1/2 Heisenberg antiferromagnet. This result found by using the simple mean-field like variational approach is indeed in agreement with findings using more advanced many-body methods [21, 24, 37].

5. Conclusions and outlook

To summarize, we have considered a mean-field like approach for the analysis of quantum phase transitions in quantum spin systems with competing antiferromagnetic bonds. This scheme can be cast into the standard Landau’s paradigm of phase transitions. Furthermore,
the method is rather transparent and simple from the calculation point of view. This method provides reasonably good estimates for quantum critical points, and the critical behaviour falls into the mean-field universality class. Because of the local character of the variational ansatz (3.1), this method cannot distinguish between various distinct patterns for the arrangement of dimers and therefore it cannot provide more refined information on the features of the quantum phase transition.

Finally, let us mention that in our review paper, except of the overview on previously published papers [21–26], we also present some new results in section 4.3. Furthermore, the illustrated variational approach can be easily applied to other systems of coupled dimers, and, thus it can be used as a simple tool to provide a better understanding of experiments on spin dimer systems (see, e.g., [38, 39]). In particular, the mean-field approach provides an estimate of the critical $J'$ for quite general geometries of coupled-dimer systems.

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