DISCONTINUOUS PHASE TRANSITION OBTAINED WITH THE THERMAL BOSON EXPANSION FOR THE HEISENBERG FERROMAGNET

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Spin waves at finite temperature of an Heisenberg ferromagnet ($S = 1/2$) have been defined in the framework of the thermal boson expansion. We analyze the discontinuous phase transition which appears when this theory of thermal magnons breaks down. Temperatures corresponding to a maximal superheating point, T_1 , a minimal supercooling point, T_0 , and a transition point, T_C , such that $T_0 \leq T_C \leq T_1$, have been identified. The temperature T_C agrees closely with the "exact" critical temperature known for the model.

Let us consider the Hamiltonian of the Heisenberg model of a $S = 1/2$ ferromagnet

$$\mathcal{H} = -J \sum_{ij} S_i \cdot S_j, \quad (1)$$

where J is the exchange integral between one localized spin and its z neighbours and S_i is the spin operator localized at the lattice point i .

The Thermal Boson Expansion (TBE) for the Hamiltonian (1) has been used for spins $S = 1/2$ in Ref. 1 and extended to spins $S \geq 1$ in Ref. 2. The same method has been applied to antiferromagnets as well.³

The method consists basically in generalizing the concept of magnons from zero temperature, when the system may be described by a pure state, to a finite temperature, when the system should be described by a mixed state. The thermal magnons are unlocalized spin deviations with respect to the temperature-dependent mean field. In that framework, a maximal temperature T_1 has been identified at which there is still a spontaneous magnetization. This temperature is far below the mean-field critical temperature, being in good agreement with the most accurate critical temperature known for the system of spins $S = 1/2$. Nevertheless, the magnetization does not vanish at that point, as is characteristic of a continuous phase transition. A re-entrant branch was found for temperatures just below T_1 . This re-entrant solution is unstable since the upper branch, which goes to the correct $T \rightarrow 0$ limit, has a lower free energy. We have a discontinuous (first-order) phase transition (for a review, see Ref. 4) although only the ferromagnetic phase can be reached with the method.

In the present letter, we examine in detail the phase transition obtained with the TBE. The maximal attainable temperature should be considered a maximal superheating temperature while, on the other hand, a minimal supercooling temperature T_0 exists at the point where the unstable magnetization branch crosses the line $M = 0$, i.e. where the unstable ferromagnetic solution, which corresponds to the line of maxima for the free energy, has the same free energy as the paramagnetic state. Between T_0 and T_1 , we may define a transition temperature T_C for which the free energies of the stable ferromagnetic solution and the paramagnetic state are equal.

After sketching the TBE, the free energy as a function of the magnetization (order parameter) and the temperature is presented. The superheating, supercooling, and transition temperatures are discussed and compared with the "exact" (most accurate value known) critical temperature.

Traditional boson expansions, which hold at zero temperature, aim at describing excitations above a ground state, which is taken to be a mean-field (or independent-particle) stationary state. A mapping of fermion or spin operators onto boson operators, such that the physics of the problem is preserved, is defined. The boson images obey the same commutation relations as the original operators and ground state expectation values are identical in both spaces.

In the TBE, this scheme is essentially maintained, but the mean-field stationary state is now taken to be a mixed state, describing a statistical situation instead of a pure state. In this way, the boson vacuum, which corresponds to the mixed state, depends on the temperature, and the excitations on this vacuum are also temperature-dependent. These are called "thermal bosons". In the context of the magnetism, the thermal mean-field is the Weiss molecular field and the bosons are thermal magnons or spin waves, whose dispersion relation depends on the temperature. This is nothing else than an extension to finite temperatures of the well-known Holstein-Primakoff expansion.⁵

We take as objects to be mapped onto boson operators the lattice Fourier transforms of the spin operators

$$S_{\mathbf{k}}^{\pm} = \frac{1}{\sqrt{N}} \sum_j e^{\pm i\mathbf{k} \cdot \mathbf{R}_j} S_j^{\pm}, \quad S_{\mathbf{k}}^z = \frac{1}{\sqrt{N}} \sum_j e^{+i\mathbf{k} \cdot \mathbf{R}_j} S_j^z. \quad (2)$$

The TBE demands that commutation relations between the operators (2) hold in the boson space, i.e.

$$[(S_{\mathbf{k}}^+)_{\mathbf{B}}, (S_{\mathbf{k}'}^-)_{\mathbf{B}}] = \frac{2}{\sqrt{N}} (S_{\mathbf{k}-\mathbf{k}'}^z)_{\mathbf{B}}, \quad [(S_{\mathbf{k}}^z)_{\mathbf{B}}, (S_{\mathbf{k}'}^{\pm})_{\mathbf{B}}] = \pm \frac{1}{\sqrt{N}} (S_{\mathbf{k}' \pm \mathbf{k}}^{\pm})_{\mathbf{B}}, \quad (3)$$

with $(S_{\mathbf{k}}^{\pm})_{\mathbf{B}}$ and $(S_{\mathbf{k}}^z)_{\mathbf{B}}$ being the bosonic images of $S_{\mathbf{k}}^{\pm}$ and $S_{\mathbf{k}}^z$ respectively. Furthermore, the conditions

$$\text{Tr}(\mathcal{D}_0 S_{\mathbf{k}}^{\pm}) = (0|(S_{\mathbf{k}}^{\pm})_{\mathbf{B}}|0), \quad \text{Tr}(\mathcal{D}_0 S_{\mathbf{k}}^z) = (0|(S_{\mathbf{k}}^z)_{\mathbf{B}}|0) \quad (4)$$

are imposed, with D_0 being the mean-field mixed state and $|0\rangle$ the boson vacuum. We take the density matrix in the form

$$D_0 = A \exp \left(\alpha \sum_j S_j^z \right), \quad (5)$$

with α being a real number. Instead of α , we prefer to use X such that

$$X = A^{1/N} \left(\exp \frac{\alpha}{2} - \exp \frac{-\alpha}{2} \right). \quad (6)$$

(The condition $\text{Tr}(D_0) = 1$ determines A). The following expansion is obtained:

$$\begin{aligned} (S_{\mathbf{k}}^+)_B &= (X)^{1/2} B_{\mathbf{k}} + \dots, \quad (S_{\mathbf{k}}^-)_B = (X)^{1/2} B_{\mathbf{k}}^+ + \dots, \\ N^{1/2} (S_{\mathbf{k}}^z)_B &= \frac{NX}{2} \delta_{\mathbf{k},0} - \sum_{\mathbf{k}'} B_{\mathbf{k}+\mathbf{k}'}^+ B_{\mathbf{k}'}, \end{aligned} \quad (7)$$

where $B_{\mathbf{k}}^+$ and $B_{\mathbf{k}}$ are creation and annihilation operators satisfying the usual commutation relations for bosons, and $B_{\mathbf{k}}|0\rangle = 0$. For the Hamiltonian, we obtain the expansion

$$(\mathcal{H})_B = -\frac{JNzX^2}{4} + \sum_{\mathbf{k}} \omega_{\mathbf{k}}(X) B_{\mathbf{k}}^+ B_{\mathbf{k}} + \dots, \quad (8)$$

with $\omega_{\mathbf{k}}(K) = Jz(1 - \gamma_{\mathbf{k}})X$, where $\gamma_{\mathbf{k}} = (1/z) \sum_l \exp(i\mathbf{k} \cdot \delta_l)$ is a structure factor (the vector δ_l goes from j to its neighbour l). The parameter X may be considered a renormalization factor of the spin waves.

We take the free energy to consist of a mean-field term and a term with the contribution of the bosonized degrees of freedom: $F = F_0 + F_2$. The first is

$$F_0 = E_0 - TS_0 = -\frac{JNzX^2}{4} + \frac{N}{\beta} \left[\log \frac{\sinh(\alpha/2)}{\sinh \alpha} + \frac{\alpha X}{2} \right], \quad (9)$$

with $\beta = (k_B T)^{-1}$ and k_B is the Boltzmann constant, while the second is

$$F_2 = E_2 - TS_2 = \frac{1}{\beta} \sum_{\mathbf{k}} \log[1 - \exp(-\beta \omega_{\mathbf{k}}(X))], \quad (10)$$

where $n_{\mathbf{k}}(X) = [\exp(\beta \omega_{\mathbf{k}}(X)) - 1]^{-1}$ are the occupancy numbers of the thermal magnons. It is impossible to have $X \rightarrow 0$ since this would mean that $n_{\mathbf{k}} \rightarrow \infty$, while a physical restriction is obviously $\sum_{\mathbf{k}} n_{\mathbf{k}} \leq N$.

The magnetization is the expectation value of the following operator

$$(M)_B = \frac{g\mu_B}{V} \left(\sum_j S_j^z \right)_B = \frac{g\mu_B f}{Na^3} \left(\frac{NX}{2} - \sum_{\mathbf{k}} B_{\mathbf{k}}^+ B_{\mathbf{k}} \right), \quad (11)$$

where g is the Landé factor, μ_B the Bohr magneton, a the lattice constant, and f a geometrical factor. The reduced magnetization is

$$\frac{M}{M_0} = \frac{M(X)}{M(1)} = X - \frac{2}{N} \sum_{\mathbf{k}} n_{\mathbf{k}}(X). \quad (12)$$

We are interested in the free energy as a function of the order parameter. Since we cannot obtain analytically the total free energy as a function of the magnetization and the temperature, $F = F(M, T)$, we must resort to numerical methods. We can indeed compute $F = F(X, T)$ and $M = M(X, T)$, obtaining the free energy as a function of the magnetization for a given temperature.

Figure 1 shows the free energy as a function of the reduced magnetization for a simple cubic lattice with $S = 1/2$ at five typical values of the temperature.

Fig. 1. The free energy as a function of the reduced magnetization for five typical values of temperature calculated for the s.c. lattice and $S = 1/2$. $F(0)$ means the free energy for $M = 0$.

We conclude that there is always a minimum of the curve $F(M, T)$, at a finite M , for $T \leq T_1$. For temperatures $T \leq T_c$, the free energy of this minimum is lower than the paramagnetic free energy $F(M = 0)$. At a temperature $T_0 < T_c$, a maximum of F exists at $M = 0$, meaning that the paramagnetic state is then an unstable stationary solution.

Following the nomenclature of first-order phase transitions, we call T_1 the maximal superheating temperature and T_0 the minimal supercooling temperature. The transition temperature T_C , intermediate between T_0 and T_1 , is obtained through the double tangent construction: at $T = T_C$, the free energy of the minimum is equal to $F(M = 0)$, i.e. the ferromagnetic and paramagnetic states have the same thermodynamic potential. We have obtained numerically the following values: $k_B T_0/3J = 0.52$, $k_B T_C/3J = 0.58$, and $k_B T_1/3J = 0.60$.

In Ref. 1, we have seen that for the system under study, the maximal attainable temperature T_1 for the ferromagnetic phase is very close to the accurate value $k_B T_C/3J = 0.56$, obtained with the aid of a high-temperature series expansion.⁶ Our present temperature T_C is slightly better than T_1 in comparison with the theoretical standard.

For describing the equilibrium free energy at a given temperature, the free energy should be varied with respect to X (this is the same as varying F with respect to the magnetization since $M = M(X, T)$). We obtain the following transcendental equation

$$X = \tanh \left\{ \frac{Jz}{2k_B T} \left[X - \frac{2}{zJN} \sum_{\mathbf{k}} \omega_{\mathbf{k}}(1) n_{\mathbf{k}}(X) \right] \right\}. \quad (13)$$

Figure 2 shows the free energy extrema as a function of temperature calculated for the s.c. lattice with $S = 1/2$. The reduced magnetization corresponding to equilibrium (stable or unstable) is presented in Fig. 3.

Fig. 2. The free energy extrema as a function of temperature calculated for the s.c. lattice with $S = 1/2$. The continuous curve represents free energy minima while the broken curve refers to free energy maxima. The phase transition temperatures T_0 , T_C , and T_1 are indicated.

Fig. 3. Reduced magnetization M/M_0 as a function of the reduced temperature calculated for the s.c. lattice with $S = 1/2$. The continuous curve represents free energy minima while the broken curve refers to free energy maxima.

These two pictures provide a good representation of the phase transition. The reduced magnetization goes from the saturation value at $T = 0$ to the value of 0.3 at the maximal temperature T_1 . The lower branch of the magnetization corresponds to maxima of the free energy. The magnetization vanishes at the temperature T_0 .

Alternative approaches for describing temperature-dependent magnons are the MRA (Magnon Renormalization Approach) proposed by M. Bloch,^{7,8} and the RPA (Random Phase Approximation).⁹ In the first method, the magnons are renormalized by the dynamical interaction while in the second, they are renormalized by the magnetization. The MRA originates a first-order phase transition similar to ours, with $k_B T_0/3J = 0.60$ and $k_B T_1/3J = 0.65$, while the RPA gives a second-order phase transition with $k_B T_C/3J = 0.66$. The limiting temperatures for the ordered phase in both methods are worst than that obtained with the TBE.

For the sake of completeness and in order to help the reader, we present the renormalization factors obtained in the MRA:

$$X = 1 - \frac{2}{JNz} \sum_{\mathbf{k}} \omega_{\mathbf{k}}(1) n_{\mathbf{k}}(X), \quad (14)$$

and in the RPA:

$$X = \left[1 + \frac{2}{N} \sum_{\mathbf{k}} n_{\mathbf{k}}(X) \right]^{-1}. \quad (15)$$

In the MRA, the magnetization is

$$\frac{M}{M_0} = 1 - \frac{2}{N} \sum_{\mathbf{k}} n_{\mathbf{k}}(X), \quad (16)$$

while in the RPA, one gets simply

$$\frac{M}{M_0} = X. \quad (17)$$

Kaplan and Stenschke¹⁰ have found a first-order phase transition in the Heisenberg ferromagnet considering the exchange integral to be dependent on the magnetization (magnetostrictive effect). A similar phenomenon has been discussed recently by Wang, Qin, and Lin¹¹ for a ferroelectric model with next neighbours interactions.

With thermal magnons, we cannot obtain a second-order phase transition, which is known to exist for the Heisenberg model, since near the transition point, fluctuations of all orders of magnitude (and not only harmonic) of the mean field play a role. Some attempts have been made to recover a second-order phase transition starting with the MRA and considering higher order interactions^{12,13} but their success have been very limited. Notwithstanding the lack of continuity of the phase transition, we think it is surprising that methods based on bosons (such as our TBE or the MRA), which are rigorous in the low temperature limit, can lead to a good prediction of the critical point for the system under study.

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