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Bose–Einstein condensation and entanglement in magnetic systems

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Abstract
We present a study of magnetic field induced quantum phase transitions in insulating systems. A generalized scaling theory is used to obtain the temperature dependence of several physical quantities along the quantum critical trajectory ($H = H_C$, $T \rightarrow 0$) where H is a longitudinal external magnetic field and H_C the critical value at which the transition occurs. We consider transitions from a spin liquid at a critical field H_{C1} and from a fully polarized paramagnet, at H_{C2}, into phases with long range order in the transverse components. The transitions at H_{C1} and H_{C2} can be viewed as Bose–Einstein condensations of magnons which however belong to different universality classes since they have different values of the dynamic critical exponent. Finally, we use that the magnetic susceptibility is an entanglement witness to discuss how this type of correlation sets in as the system approaches the quantum critical point along the critical trajectory, $H = H_{C2}$, $T \rightarrow 0$.

1. Introduction

Recently there has been an intense study of field induced quantum phase transitions in metallic [1–6] and insulating materials [7–12]. These field induced transitions are generally associated with a Bose–Einstein condensation of magnons. In the insulating case, most of the experimental studies have concentrated in obtaining the *shift exponent* that characterizes the shape of the critical line in the neighbourhood of the quantum critical point (QCP). However, it is important to have additional experimental information that can be used to fully characterize the universality classes of the different zero temperature field induced transitions. For this purpose it is convenient to obtain the thermodynamic behaviour of the system along a special trajectory in the phase diagram. This *quantum critical trajectory* consists essentially in *sitting* at the quantum critical point, by fixing the magnetic field at its critical value and varying the temperature. Field induced transitions are generally associated with soft modes. Then, at the QCP where the gap for excitation vanishes, physical quantities such as specific heat, magnetization and susceptibility have power law temperature dependences determined by the quantum critical exponents. Our aim here is to obtain this behaviour. This strategy has been intensively explored in the study of heavy fermion materials, in this case, fixing the pressure at its critical value for the disappearance of magnetic order [13]. This approach is particularly useful for insulating materials where the magnons that become soft at the QCP account for most of the low temperature thermodynamic behaviour. In metals, even in field induced transitions, one has to consider also the contribution of charge carrying excitations [1–6]. The soft magnon modes couple to these excitations and both may be strongly renormalized.

We will consider two types of field induced transition. First, we study the zero temperature transition in an antiferromagnet system, from the fully polarized paramagnetic state into a phase with transverse components of the magnetization as the longitudinal magnetic field is *reduced* to a critical value H_{C2} [14]. This is a second order transition which is characterized by a dynamic critical exponent $z = 2$ [14]. It can be identified with a Bose–Einstein condensation of magnons with the magnetic field playing the role of the chemical potential. We also consider the transition from a disordered spin-liquid phase to an antiferromagnetic phase [11], at a critical magnetic field, H_{C1}. In this case the field is increased to the critical value H_{C1} at which the singlet gap vanishes and magnetic long range order sets in. This transition is characterized by a dynamic critical exponent $z = 1$ [15]. In both cases the transition is approached from the *disordered* side, i.e., with $H > H_{C2}$ and $H < H_{C1}$. Although these transitions have been intensively studied [9–12, 16], the physical behaviour along the quantum critical trajectory, $H = H_C$, $T \to 0$, has not been sufficiently characterized. In this paper we fully determine the thermodynamic properties and the appearance of entanglement along this line. We hope in this way to motivate further experiments that go beyond obtaining the shift exponent of the critical line. Notice that, away from the QCP, in the disordered phase, the excitations are gapped and the physical behaviour is thermally activated.

Our results are obtained using a generalized quantum scaling theory which was previously applied to heavy fermion materials [17, 18]. This theory describes completely the thermodynamic behaviour along the quantum critical trajectory. The reason is that we consider three dimensional materials and the effective dimensions [17, 18] at the field induced quantum phase transitions $d_{\mathrm{eff}} = d + z$ are at, or above, the upper critical dimension $d_c = 4$ for these transitions. In this case, the quantum critical exponents assume Gaussian or mean-field values, being fully determined. Logarithmic corrections which arise in the case $d_{\mathrm{eff}} = d_c$ are not obtained in the present approach. The microscopic justification of the scaling theory is provided by renormalization group calculations [19, 16]. In the last section we discuss how entanglement sets in among the spins along the quantum critical trajectory.

2. Scaling analysis of the quantum phase transition

We consider first an antiferromagnetic system with longitudinal anisotropy and a strong magnetic field applied along the easy axis direction. We study the $T = 0$ transition, with decreasing magnetic field, from the fully polarized paramagnet to a phase with long range order in the transverse components of the magnetization at a critical field $H_{C2}(T = 0)$ [14]. This problem can be treated as a dilute gas of bosons with the effective action given by [16]

$$S = \frac{1}{2}\int_{\mathbf{k},\omega} [\mathrm{i}\omega + Dk^2 + \delta]|\psi(\mathbf{k},\omega)|^2 + v_0 \int_{\mathbf{x},\tau} |\psi|^4 \qquad (1)$$

where $\delta = H - H_{C2}$. The field $\psi(\mathbf{k}, \omega)$ is a two-component field representing the components of the spins transverse to the direction of the magnetic field and v_0 takes into account the spin–wave interactions. The transition at $\delta = 0$ has a dynamic exponent $z = 2$ due to the ferromagnetic-like dispersion of the magnons [14]. This action has been extensively studied in the context of the non-ideal Bose gas [20], the dilute Bose gas [21] and superfluid–insulator transitions [22]. In our case it is useful due to the small number of magnons excited at the field induced quantum phase transition [23]. It takes into account the ferromagnetic-like dispersion of these modes [14] and incorporates a constraint in their total number [23].

The thermodynamic properties of systems, close to the QCP described by the action in equation (1), can be obtained from the free energy density. This has the scaling form[1]

$$f \propto |\delta(T)|^{2-\alpha} F\left(\frac{T}{|\delta(T)|^{\nu z}}\right) \tag{2}$$

near the QCP. The zero temperature critical exponents α, ν and the dynamic exponent z are related to the dimensionality of the system d by the quantum hyperscaling relation, $2-\alpha = \nu(d+z)$ [18]. In general for $d_{\mathrm{eff}} = d+z > 4$, i.e., above the upper critical dimension $d_{\mathrm{c}} = 4$, the exponents associated with the QCP at $\delta = 0$ take Gaussian values, and in particular the correlation length exponent, $\nu = 1/2$. For the action in equation (1) these exponents remains Gaussian even below $d_{\mathrm{c}} = 2$ [20]. Although within the renormalization group approach for $d = 3$ the transition at $\delta = 0$ is controlled by the Gaussian fixed point, the spin–wave coupling v_0 acts as a *dangerously* irrelevant interaction for $d_{\mathrm{eff}} > 4$, and must be dealt with carefully [19]. Perturbation theory in powers of v_0 leads to a temperature dependent critical line given by $\delta(T) = H_{\mathrm{C2}}(T) - H_{\mathrm{C2}} + v_0 T^{1/\psi} = 0$ with the shift exponent $\psi = z/(d+z-2) = 2/3$ in three dimensions [19].

In order to obtain the correct scaling behaviour near the QCP, the scaling function $F(x)$ in equation (2) must have the asymptotic behaviour

$$F(x) = \begin{cases} \text{constant} & \text{for } x \to 0 \\ x^p & \text{for } x \to \infty. \end{cases} \tag{3}$$

The first guarantees that we recover the correct behaviour at $T = 0$, with $f \propto |\delta|^{2-\alpha}$. The second, with $p = (\tilde{\alpha} - \alpha)/\nu z$, yields

$$f(T) \propto A(T)|\delta(T)|^{2-\tilde{\alpha}} \tag{4}$$

where $A(T) = T^p$ (see footnote 1). *Tilde* exponents refer to finite temperature transitions and $\tilde{\alpha}$ is the Gaussian thermal specific heat exponent of the three-dimensional XY model. This is related to the thermal Gaussian correlation length exponent $\tilde{\nu}$ through the Josephson relation, $2-\tilde{\alpha} = \tilde{\nu}d$. Since $\nu = \tilde{\nu} = 1/2$ for $d+z > 4$, the free energy in the neighbourhood of the QCP can be written as $f \propto T|\delta(T)|^{\tilde{\nu}d}$ ($p = 1$). From this expression we obtain the temperature dependence of the magnetization, susceptibility and specific heat at $H = H_{\mathrm{C2}}$,

$$m = a_1 T^{3/2} + b_1 v_0^{1/2} T^{7/4} \tag{5a}$$

$$\chi = a_2 T^{1/2} + b_2 (1/v_0)^{1/2} T^{1/4} \tag{5b}$$

$$C_V = a_3 T^{3/2} + b_3 v_0^{3/2} T^{9/4} \tag{5c}$$

respectively, where the (a_i, b_i) are constants. For each quantity, the first term is the Gaussian contribution and the second arises from corrections due to the dangerous irrelevant spin–wave interaction v_0. Notice that, except for the susceptibility and correlation length (see table 1), for which v_0 behaves as a truly dangerously irrelevant interaction as it appears in a denominator, the purely Gaussian term is dominant at low temperatures. A similar analysis can be carried out for the transition from the spin liquid to the antiferromagnet at H_{C1} with a dynamic exponent $z = 1$. The results are given in table 1. This case is *marginal*, since $d_{\mathrm{eff}} = d_{\mathrm{c}} = 4$ is the upper critical dimension and there are logarithmic corrections to the quantities in table 1. These however are not obtained in the scaling approach (see [15, 24]).

[1] See [18] p 20 and 106.

Table 1. Power law temperature dependence of physical quantities along the critical trajectory ($H = H_C$, $T \to 0$). Logarithmic corrections are not included. Only the dominant contribution in the low T limit is given[2] [25].

Physical quantity		$H_{C1}(z = 1)$	$H_{C2}(z = 2)$
Shift exponent	$\psi = \frac{z}{d+z-2}$	$1/2$	$2/3$
Magnetization	$-\partial f/\partial H$	T^2	$T^{3/2}$
Susceptibility	$-\partial^2 f/\partial H^2$	$\frac{1}{\sqrt{v_0}}$	$\frac{1}{\sqrt{v_0}} T^{1/4}$
Specific heat	$-T\partial^2 f/\partial T^2$	T^3	$T^{3/2}$
Correlation length	$\frac{1}{\sqrt{v_0}} T^{-\nu/\psi}$	$\frac{1}{\sqrt{v_0}} T^{-1}$	$\frac{1}{\sqrt{v_0}} T^{-3/4}$

Away from the QCP, for $H > H_{C2}$ and $H < H_{C1}$, there are gaps for excitation of spin waves and the crossover temperature $T_\times \propto |\delta|^{\nu z}$ gives the energy scale for the thermally activated behaviour of the thermodynamic functions in these regions of the phase diagram. Since these gaps vanish as $|\delta|^{\nu z}$ their measurement allows for a determination of the gap exponent νz. Notice that the difference in universality classes of the two transitions studied above arises essentially from the different dispersion relations of the soft magnons at the QCP.

Finally, at $T = 0$ in the ordered phase, it is also necessary to take into account the dangerous irrelevant spin–wave interaction v_0. The scaling form of the free energy is [18], $f \propto |\delta|^{\nu(d+z)} F_v \left[v_0|\delta|^{(d+z-4)/2}\right]$. The dangerous irrelevant nature of v_0 is manifested in the fact that the scaling function $F_v[x \to 0] \propto 1/x$. This yields

$$f \propto \frac{|\delta|^{\nu(d+z)}}{v_0|\delta|^{(d+z-4)/2}} = \frac{|\delta|^2}{v_0}$$

for $d + z > 4$. This mean-field behaviour gives rise to a *longitudinal* magnetization varying linearly with the distance to the QCP, i.e., $M \propto |H - H_C|$.

3. Entanglement and the quantum phase transition

Recently, there has been a large interest in characterizing entanglement in systems near quantum critical points and in macroscopic magnetic systems [26]. For a system with N spins, Wiesniak *et al* [27] have shown that the magnetic susceptibility acts as an entanglement witness, and that whenever

$$\tilde{\chi} = \chi_x + \chi_y + \chi_z \leqslant \frac{Nl}{kT} \tag{6}$$

there is entanglement between the individual spins of magnitude l. The χ_i are the susceptibilities along three orthogonal axis measured in the same quantum state. A quantum complementarity relation involving the susceptibility and magnetization can also be obtained [27] ($T \neq 0$),

$$1 - \frac{kT\tilde{\chi}}{Nl} + \frac{M^2}{N^2 l^2} \leqslant 1. \tag{7}$$

This is particularly useful when applied to low dimensional materials, or systems at quantum criticality, as the temperature can be reduced without any phase transition. In the equation above, it is useful to define the quantity $E(T, H) \equiv 1 - (kT\tilde{\chi})/Nl$ which provides a measurement of entanglement, while the last term $S \equiv M^2/N^2l^2$ represents local properties. Equation (7) shows the interplay between these quantities, since $0 \leqslant E + S \leqslant 1$.

[2] For $z = 2$ similar results have been obtained for a metallic antiferromagnet near H_{C2} by Fischer and Rosch [25].

It is interesting to apply the relations above to the previous problems. Let us consider the case $z = 2$, with the applied magnetic field fixed at the critical value H_{C2}. For $T = 0$ and $H \geqslant H_{C2}$ the system is in a fully polarized state, $M = Nl$, and we must have $E(T \to 0, H = H_{C2}) \to 0$. This implies that, as $T \to 0$, $\tilde{\chi} = \chi_x + \chi_y + \chi_z = Nl/kT$. Since the system is already fully polarized at $T = 0$, we must have $\chi_z(T \to 0, H = H_{C2}) \to 0$ and, consequently, $\chi_x(T \to 0, H = H_{C2}) = \chi_y(T \to 0, H = H_{C2}) = Nl/2kT$. Assuming that the transverse uniform susceptibilities have already taken their low temperature asymptotic behaviour as entanglement sets in with decreasing temperature, an approximate condition for the appearance of this type of correlation can be obtained from equation (6) in terms of the longitudinal susceptibility alone. This is given by $\chi_z < Nl/2kT$. For the specific case that the spin $l = 1$, this condition can be made precise [28]. It turns out that whenever $\chi_z(T, H = H_{C2}) < (9/16)(N/kT)$, entanglement sets in among the spins.

As temperature increases along the line $H = H_{C2}$, the entanglement measure $E(T)$ also increases. Since the magnetization for $H = H_{C2}$ decreases as $M = Nl(1 - aT^{3/2})$, the complementarity relation equation (7) implies that

$$E(T) = 1 - \frac{kT\chi}{Nl} \leqslant 1 - (1 - aT^{3/2})^2. \tag{8}$$

This can be written as $E(T) \leqslant f(T/T_C)$, where $T_C = (1/a)^{2/3}$. The quantity a is easily calculated and we get ($l = 1$)

$$T_C = \frac{1}{\zeta(3/2)^{2/3}} \frac{2\pi\hbar^2}{mk_B} \frac{1}{v^{2/3}}. \tag{9}$$

This is just the Bose–Einstein condensation temperature of a system of N bosons. In this expression, $m = (\hbar^2/2D)$ is the mass of the magnons with spin-wave stiffness D and $v = V/N$, with N the total number of spins in the volume V. In our problem described by equation (1) this arises due to the constraint in the number of modes and that the dominant contribution for the decay of the magnetization is the Gaussian one, the interaction v_0 being truly irrelevant for this quantity (see table 1). Thus at low temperatures where the spin-wave approximation holds entanglement scales with the characteristic temperature T_C at the quantum critical point. This is an interesting feature of this quantum phase transition associated with a soft mode. Although the crossover temperature $T_\times \propto |\delta|^{\nu z}$ vanishes at the QCP and excitations become gapless, the mass of the bosons remains finite, providing an energy scale even at the QCP.

It is useful to explore the analogy of the present magnetic problem with a true Bose–Einstein condensation of bosonic particles [29] to gain insight in the latter problem. The relevant Bose–Einstein transition in this case is the zero temperature density-driven transition in a system of interacting bosons from the incompressible insulating phase to the superfluid [22, 23, 30]. The control parameter δ is given by $\mu - \mu_C$, where μ_C is the critical (interaction dependent) value of the chemical potential. The magnetization in the magnetic problem corresponds to the number of condensed bosons and the longitudinal susceptibility to the compressibility defined as $\kappa = -\partial^2 f/\partial\mu^2$. The transverse uniform susceptibility can now be associated with the order parameter susceptibility of the superfluid [29] and diverges for $T \to 0$ at the QCP[3], $\mu = \mu_C$. The analogy with the magnetic case yields a criterion for the appearance of entanglement along the quantum critical trajectory ($\mu = \mu_C, T \to 0$) that can be expressed solely in terms of the compressibility. For $l = 1$, this is given by $\kappa < (9/16)(N/kT)$.

[3] The nature of the transverse order in the magnetic problem, either ferromagnetic or antiferromagnetic, is irrelevant [23] as their QCPs are in the same universality class. However, it is more useful to carry on the analogy of the Bose–Einstein problem with the ferromagnet, since in this case the uniform transverse susceptibility is the order parameter susceptibility with well defined scaling behaviour at the QCP.

The characteristic temperature which constrains the entanglement measure is the Bose–Einstein critical temperature of bosons with density $n(\mu_C)$. Entanglement in this case implies the establishment of phase coherence among the particles [29].

4. Conclusions

We have obtained the thermodynamic properties at the quantum critical point of magnetic field induced phase transitions using a scaling approach. We considered first the zero temperature transition from the saturated paramagnetic phase to a phase with long range order in the transverse components of the magnetization with decreasing field. We also presented results for the field induced transition from the spin liquid to the antiferromagnet. These transitions are in different universality classes, due to the distinct values of the dynamic critical exponents. These are determined by the dispersion relation of the gapless excitations at the QCP. Since for three-dimensional systems and the dynamic exponents considered here $d_{\mathrm{eff}} \geqslant d_{\mathrm{c}}$, the critical exponents associated with both QCPs can be immediately obtained in this case. Although for $d_{\mathrm{eff}} \geqslant d_{\mathrm{c}}$ the fixed point governing the quantum phase transition is Gaussian, in both cases, the quartic term in the action due to spin–wave interaction is dangerously irrelevant and must be considered. It plays a fundamental role in determining the critical line and the behaviour along the quantum critical trajectory of the correlation length and susceptibility.

For the problem described by the action equation (1), the zero temperature exponents remain Gaussian even below $d_{\mathrm{c}} = 2$ [20]. However, as discussed below equation (4), the behaviour along the quantum critical trajectory in the presence of dangerously irrelevant interactions it is also affected by the thermal exponents. For this reason we restricted our analysis to three-dimensional systems. Finally, we have investigated entanglement properties along the critical line as witnessed by the magnetic susceptibility. We have shown that, at the QCP, the Bose–Einstein condensation temperature provides a well defined energy scale for the appearance of entanglement among the spins.

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