Remarks on quantum critical behavior in heavy fermions

Mucio A. Continentino
Instituto de Física - Universidade Federal Fluminense
Av. Litorânea s/n, Niterói, 24210-340, RJ - Brazil
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Generalized scaling relations and renormalization group results are used to discuss the phase diagrams of heavy fermion systems. We consider the cases where these materials are driven to a magnetic quantum critical point either by applying external pressure or a magnetic field. The Ehrenfest equation relating the pressure derivative of the critical temperature to the ratio of thermal expansion and specific heat close to a magnetic quantum critical point (QCP) is analyzed from the scaling point of view. We consider different phase diagrams of antiferromagnetic heavy fermions in an external uniform magnetic field and the implication of renormalization group results for predicting their behavior.

Scaling theories are invaluable tools in the theory of quantum critical phenomena. Although these theories do not predict the values of the critical exponents, they yield relations among them. Besides they show the relevant physical quantities to be measured and the exponents that can be extracted from their critical behavior. In the case of heavy fermion systems, where there is no clear microscopic theory yet for their quantum criticality, the scaling approach is specially useful [1]. In this Report, we use a generalized scaling theory of heavy fermions [1] near an antiferromagnetic quantum instability to obtain some useful and general relations involving measurable physical quantities and the exponents that control their critical behavior. We start considering the case in which criticality is tuned by pressure and next the effects of an external magnetic field.

The Ehrenfest relation [2] when applied to magnetic systems close to a zero temperature magnetic instability is a useful thermodynamic relation. This equation that relates the pressure derivative of the line of critical temperatures, \( T_N \) to thermodynamic quantities at the quantum critical point (QCP) can be written as [2],

\[
\frac{dT_N}{dP} = T \frac{\Delta \beta}{\Delta C} = V \frac{\Delta \beta}{\Delta C/T}
\]

(1)

where \( \Delta \beta \) and \( \Delta C \) are the differences in thermal expansion and specific heat in the two phases (the critical part), respectively. The thermal expansion is defined by

\[
\beta = \frac{1}{V} \frac{\partial V}{\partial T} = -\kappa_T \frac{\partial^2 F}{\partial T \partial V}
\]

(2)

with the isothermal compressibility \( \kappa_T = -\frac{1}{V} \frac{\partial V}{\partial T} \). The volume thermal expansion, \( \beta = 2\alpha_a + \alpha_c \) where \( \alpha_a \) are the linear thermal expansion coefficients along different axes \( i \).

The expression for the critical line of finite temperature phase transitions close to the QCP is written as [3],

\[
T_N \propto |V - V_c|^{\psi} \propto |P - P_c|^{\psi}
\]

which defines the shift exponent \( \psi \). We have assumed that the critical temperature of the phase transition is reduced by changing the volume, for example, by applying pressure in the system. The quantities \( V_c \) and \( P_c \) are the critical volume and pressure, respectively. From the equation above we obtain,

\[
\frac{dT_N}{dP} \propto |P - P_c|^{\psi - 1} \propto T_N^{1 - \frac{1}{\psi}}.
\]

(3)

In the usual theory of quantum spin density wave transitions [4] the shift exponent can be expressed in terms of the dynamic exponent \( z \) and the dimensionality of the system \( d \), for \( d + z > 4 \), as \( \psi = z/(d + z - 2) \), in which case we get,

\[
\frac{dT_N}{dP} \propto |P - P_c|^{\psi - 1} \propto T_N^{\frac{4 - d}{d + z}}
\]

(4)

Equation (3) can be also obtained using the Ehrenfest relation and the generalized scaling form of the singular part of the free energy density which is given by [3],

\[
f \propto A(T)|V - V_c - uT^{1/\psi}|^{2 - \tilde{\psi}}
\]

(5)

where

\[
A(T) = T^{\tilde{\alpha} - \alpha}
\]

In these equations, the tilde exponents are associated with the finite temperature phase transition and the non-tilde with the quantum critical point, since in general these transitions are in different universality classes [3].

For the coefficient of thermal expansion, we get

\[
\Delta \beta(V = V_c) \propto \frac{\partial^2 f}{\partial T \partial V}|_{V = V_c} \propto u^{1 - \tilde{\alpha}} T^{-\frac{\tilde{\alpha} - \alpha}{\psi}} - 1 + \frac{1 - \tilde{\alpha}}{\psi}
\]

(6)

For the specific heat we get [3],

\[
\Delta C/T |_{V = V_c} \propto \frac{\partial^2 f}{\partial T^2}|_{V = V_c} \propto u^{2 - \tilde{\alpha}} T^{-\frac{\tilde{\alpha} - \alpha}{\psi}} + \frac{2 - \tilde{\alpha}}{\psi}
\]

and finally we obtain for the ratio [3, 3, 3],

\[
\frac{\Delta \beta}{\Delta C/T} |_{V = V_c} \propto \frac{u^{1 - \tilde{\alpha}} T^{-\frac{1 - \tilde{\alpha}}{\psi}} - 1}{u^{2 - \tilde{\alpha}} T^{-\frac{\tilde{\alpha} - \alpha}{\psi}} - 2} = \frac{1}{u^{\frac{1}{\psi} - 2}}
\]

(7)
in agreement with Eq. 1. This is a general scaling result but in the theory of quantum spin-density wave transitions, for \( d + z > 4 \), the quantity \( u \) can be identified as the dangerous irrelevant quartic interaction \( \mathcal{A} \) of the action \( \mathcal{S} \). Notice that working from the paramagnetic side of the quantum critical point, the relevant exponent which governs the ratio above is the crossover exponent \( \nu z \). This seems to imply the scaling relation \( \psi = \nu z \) which identifies the shift with the crossover exponent. Eq. 1. The spin density wave theory \( \mathcal{S} \) makes clear the role of the dangerous irrelevant variable \( u \) in the violation of this scaling relation. Then the ratio given by Eq. refratio, in a system which is driven to a quantum critical point by pressure, provides information on the shift exponent of the critical line. For a spin-density wave transition at \( d + z > 4 \), it depends explicitly in the dangerous irrelevant variable \( u \).

We now investigate the effects of a magnetic field in the phase diagram of antiferromagnetic heavy fermion systems \( \mathcal{S} \). We consider Ising-like systems with strong anisotropy and exclude from our discussion the cases of phase diagrams with bicritical points. The main effect of the field that concerns us here is that, when sufficiently strong, it can drive the transition temperature to zero. We discuss two different types of phase diagrams.

The most simple situation is that shown in Fig. 1 where the magnetic field is a completely irrelevant variable in the RG sense. From the expected flow of the RG equations \( \mathcal{S} \) shown in Fig. 1 we find that if the system leaves the AF phase by increasing the magnetic field at finite \( T \), the relevant exponents are those of the finite temperature, zero field Néel transition \( \mathcal{S} \). On the other hand if the system is driven, at zero temperature, to the paramagnetic phase by increasing the field, the relevant exponents are those of the zero field quantum critical point at \((J/W)_c\) or \( \mathcal{P}_c \). Here \((J/W)\) is the usual ratio between the Kondo lattice parameters \( \mathcal{S} \). In this case, the critical line close to the PCQ vanishes as \( \mathcal{H}_c \propto (J/W) - (J/W)_c \) with an analytic field dependence \( \mathcal{S} \).

A more interesting case is that of Fig. 2. Now there is a line of tricritical points \( (t) \mathcal{S} \), see Fig. 2 separating the lines of first and second order phase transitions that merges with the \( H = 0 \) quantum critical point \( \mathcal{S} \). An essential feature in this case is that the magnetic field at the zero temperature line \( (H_c) \) containing the end points of the lines of first order transitions scales as \( h' \propto h^d \), where \( h \) is the scaling factor, \( d \) the dimension of the system and \( h = H - H_c \). The reason is that at this line the magnetic field has to reverse a large number of spins of the order of the volume of the sample. Notice that this special line does not include the multicritical point at \( H = 0 \). The concept of finite size scaling \( \mathcal{S} \), with the inverse of temperature \( T \) playing the role of a cut-off length, \( L_r = T^{-1/2} \), and the scaling exponent of the magnetic field obtained before yields the scaling form for the free energy at small but finite temperatures close to the line \( \mathcal{H}_c(J/W) \) or \( \mathcal{H}_c(P) \),

\[
\mathcal{F} \propto |h| \mathcal{F}\left(\frac{T}{|h|^z/d}, \frac{T}{|h|^z/d}\right)
\]  (8)

from which the thermodynamic quantities can be obtained. The scaling function \( \mathcal{F}(0) = \text{constant} \) to allow for a discontinuity in the magnetization at zero temperature as the line of first order transitions is crossed. The effects of couplings to dangerous irrelevant variables may be taken into account defining

\[
h = H - H_c - uT^{1/\nu_h},
\]
where in mean field $\psi_H = 1/2$ or with another exponent to describe the $H_c$ dependence of $(J/W)$. Notice that this is the situation expected for a highly anisotropic, Ising-like material. Notice that this is the situation expected for a highly anisotropic, Ising-like material. Notice that the scaling expression, Eq. 8, is useful for systems with a finite $T_N$ which are driven to a quantum critical point by the effect of an applied magnetic field. It does not apply at the quantum multicritical point at $H = 0$.

We have pointed out important consequences of the application of Ehrenfest relation to antiferromagnetic materials close to a quantum critical point. Generalized scaling relations were necessary to describe the system close to the QCP where the Néel temperature vanishes. We have used some well known results from the phase diagram and renormalization group studies of antiferromagnetic systems in a magnetic field to investigate the effects of this field in the field-driven magnetic instability at zero temperature which may be realized, for example, in heavy fermion systems.

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\[ \text{* Electronic address: mncio@if.uff.br} \]