Landau theory of compressible magnets near a quantum critical point

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Landau theory is used to investigate the behavior of a metallic magnet driven toward a quantum critical point by the application of pressure. The observed dependence of the transition temperature with pressure is used to show that the coupling of the magnetic order to the lattice diverges as the quantum critical point is approached. This means that a first order transition will occur in magnets (both ferromagnets and antiferromagnets) because of the coupling to the lattice. The Landau equations are solved numerically without further approximations. There are other mechanisms that can cause a first order transition so the significance of this work is that it will enable us to determine the extent to which any particular first order transition is driven by coupling to the lattice or if other causes are responsible. © *2010 American Institute of Physics*. [doi:10.1063/1.3366612]

I. INTRODUCTION

A quantum critical point (QCP) is approached by applying pressure in a number of conducting ferromagnetic and antiferromagnetic metals.[1–3] This involves a transition from a magnetic metal to a phase that is a strongly correlated Fermi liquid. In some cases, a superconducting phase appears as the QCP is approached, however, in a number of materials, a first order transition occurs just before the QCP is reached.[4] The observed dependence of T_c on pressure necessarily means that the magnetic energy is coupled to the lattice. A first order phase transition occurs if this coupling exceeds a critical value. This is inevitable if the pressure derivative of T_c diverges at the QCP as occurs for metallic materials[5] for which a power law dependence is found for the dependence of the transition temperature on pressure $T_c(p) = T_0[1 - (p/p_0)]^\eta$, where $\eta < 1$. There are good theoretical arguments for expecting that $\eta = 3/4$ (Ref. 6) so we shall use this value in what follows. The temperature and magnetic field behavior of many of the weak metallic magnets e.g., $ZrZn_2$ are described very well by Landau theory over a wide parameter range so it is useful to use this approach to get the whole phase diagram.

The physics of the problem is understood from the fact the magnetostriction will expand the lattice in the ordered phase when the transition temperature falls when the material is compressed. This leads naturally to a first order phase transition because we can reach a pressure where the transition temperature in the paramagnetic phase is above the ambient temperature but because of magnetostriction the strain in the ordered phase is reduced so the transition temperature drops sufficiently so that the ordered phase is stable. Thus there is a mixed phase region consisting of nonmagnetic and magnetic regions. The magnetization is also enhanced in the second order regime because the magnetic energy is enhanced below the ordering temperature due to the magnetostriction.

Both the magnetization and hence the magnetostriction vanish at the critical temperature of a second order transition and so the transition temperature may be defined in terms of the strain, $T_c(\varepsilon) = T_0[1 - (\varepsilon/\varepsilon_0)]^{3/4}$, where $\varepsilon_0 = p_0/K$ and K is the elastic modulus. This is the expression used to write the strain in the material in terms of the strain due to the applied pressure which is present in the paramagnetic phase, $\varepsilon_s = p/K$ and the additional strain due to magnetostriction. This generates a coupling between the square of the order parameter and the magnetostrictive strain.

II. LINEAR THEORY

The Landau free energy of a magnetic material, including the hydrostatic pressure, for which the transition temperature, T_c is a function of the strain ε, is written as follows:

$$F(M,\varepsilon;p,T) = \frac{A}{2}(T - T_c(\varepsilon))\mathbf{M}^2 + \frac{B}{4}(\mathbf{M}^2)^2 + \frac{C}{6}(\mathbf{M}^2)^3$$

$$+ O(M^8) + \frac{K\varepsilon^2}{2} - p\varepsilon \qquad (1)$$

In the paramagnetic phase, the equilibrium value of the strain is given by $\varepsilon_s = p/K$. In the linearized theory, T_c is expanded about ε_s to first order, $T_c(\varepsilon) = T_c(\varepsilon_s) + \{[\partial T_c(\varepsilon)]/(\partial \varepsilon)\}|_{\varepsilon = \varepsilon_s}(\varepsilon - \varepsilon_s)$.

The free energy is minimized with respect to $(\varepsilon - \varepsilon_s)$ and this produces a renormalization of the fourth order coefficient,

$$B' = B\left(1 - \frac{2\zeta^2}{KB}\right), \quad \text{where} \quad \zeta = \frac{A}{2} \left. \frac{\partial T_c(\varepsilon)}{\partial \varepsilon}\right|_{\varepsilon = \varepsilon_s} \qquad (2)$$

The tricritical point occurs where B' goes to zero. The enhancement of the magnetization in the ordered phase, mentioned earlier occurs because of the reduced value of B. The magnetization is evaluated as a function of temperature for the second order and tricritical regimes in this model in order to compare it with the self-consistent theory described below. Although this theory does give a first order region the value
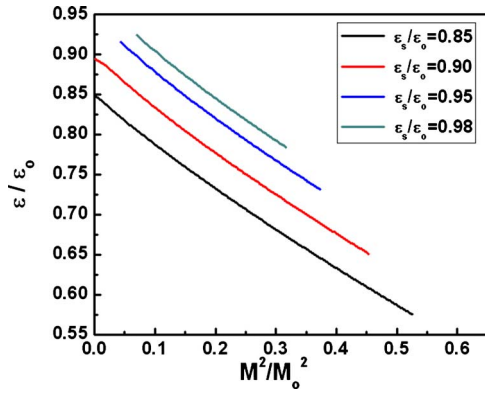

FIG. 1. (Color online) The change in the strain with magnetization. The QCP occurs for the strain ε_0 and the strain in the absence of magnetization is ε_s and the magnetization is normalized by $M_0^2 = (AT_0)/B$.

FIG. 2. (Color online) The change in the transition temperature with magnetization caused by the change in the strain.

of the magnetization in the ordered phase is unreasonably high.

III. SELF-CONSISTENT THEORY

In the case that the reduction in the transition temperature follows a power law as a function of strain or pressure as is seen in metallic materials, a more complete theory can be used.[5] The minimum of the free energy (1) is given by the solution of the two equations,

$$\frac{\partial F(M,\varepsilon;p,T)}{\partial M} = 0 = M\{A[T - T_c(\varepsilon)] + B\mathbf{M}^2 + O(M^4)\},$$

(3)

$$\frac{\partial F(M,\varepsilon;p,T)}{\partial \varepsilon} = 0 = -\frac{A}{2}\frac{\partial T_c(\varepsilon)}{\partial \varepsilon}\mathbf{M}^2 + K\varepsilon - p,$$

(4)

the solutions are: $M = 0$ or $M^2 = \frac{A[T_c(\varepsilon) - T]}{B}$, (5)

$$\varepsilon = \frac{p}{K} + \frac{A^2}{2BK}[T_c(\varepsilon) - T]\frac{\partial T_c}{\partial \varepsilon}.$$

(6)

We solve these equations numerically using $T_c(\varepsilon) = T_0(1 - \varepsilon/\varepsilon_0)^{3/4}$. In the nonmagnetic phase, the strain takes the temperature independent value, $\varepsilon = \varepsilon_s = p/K$. The parameters were chosen such that the tricritical point occurs for $\varepsilon_s/\varepsilon_0 = 0.9$. In Fig. 1 we show the dependence of the strain with the magnetization as calculated from Eq. (3). The magnetization is divided by a normalization factor, $M_0^2 = (AT_0)/B$, which is the value of the saturation magnetization when T_c is independent of strain. When $M = 0$ the strain takes the value $\varepsilon = \varepsilon_s$ but for finite magnetization the strain is always below this value in some cases by a very significant amount. The curves are only drawn for the range of magnetization that actually occurs for that value of the applied strain. Since the transition temperature depends on the strain, we can combine the results shown in Fig. 1 to calculate the dependence of the transition temperature on the magnetization and this is plot-
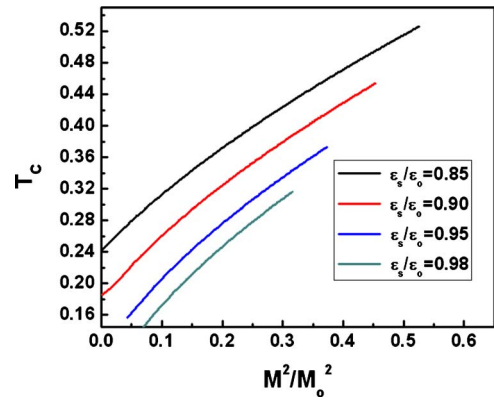
ted in Fig. 2. This shows the expected effect that T_c increases with the magnetization; but we see from Eq. (3) that an increase in T_c leads in turn to an increase in the magnetization. It is this positive feedback that leads to a first order transition. Near to the QCP the transition temperature is a very sensitive function of the strain and so the linear theory is valid only when the magnetization is very small and hence this theory is valid over a very narrow temperature range.

This is shown in Fig. 3 which shows the temperature dependence of the strain obtained from the self-consistent solution of Eq. (4). There are three different types of curves shown; in all cases $\varepsilon < \varepsilon_s$ because $[\partial T_c(\varepsilon)]/(\partial\varepsilon) < 0$. For $\varepsilon_s/\varepsilon_0 < 0.9$, in the second order region, the curve of $\varepsilon/\varepsilon_0$ approaches the value of $\varepsilon_s/\varepsilon_0$ smoothly. At the tricritical point, the curve of $\varepsilon/\varepsilon_0$ approaches $\varepsilon_s/\varepsilon_0$ with a vertical slope, this arises because of the tricritical exponents. For higher pressure, in the first order region, the curves are discontinuous, what is shown here is the point where the ordered phase becomes unstable—there is another, lower, temperature where the paramagnetic phase is unstable and there is a mixed phase between these points.[5] The pressure dependence of the transition temperature is clear from the temperatures at which the curves terminate for different values of ε_s. Since $T_c(\varepsilon)$ is a strong function of ε the reduction of ε in the ordered phase acts to increase T_c which in turn increases M as is seen from Eq. (3). The magnetization is given by plots shown in Figs. 4 for the second order and tricritical regimes.
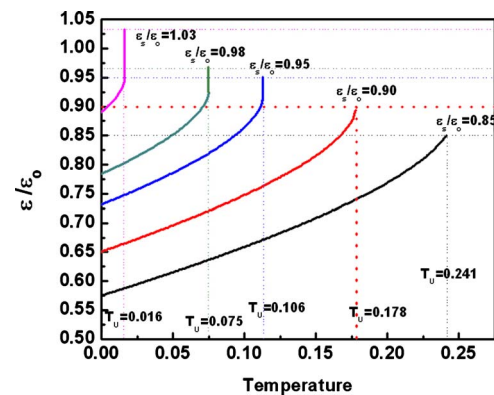

FIG. 3. (Color online) The strain in the magnetic phase from Eq. (4), the self-consistent theory, the tricritical point occurs for $\varepsilon_s/\varepsilon_0 = 0.9$.
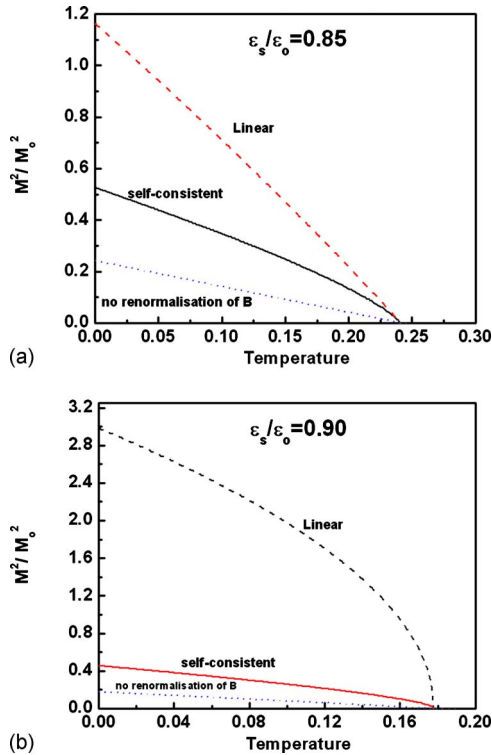
FIG. 4. (Color online) The magnetization as a function of temperature in (a) the second order region and (b) at the tricritical pressure; a comparison of the linear and self-consistent theory.

FIG. 5. (Color online) The magnetization as a function of temperature for different pressures.

IV. CONCLUSIONS

We have shown that the linear theory, which is defined to be valid just near the transition, gives results that deviate substantially from the self-consistent calculation at low temperatures in the second order regime and in the first order regime. We have shown that the effects of the coupling to the lattice are strongest in the region of the transition but then are reduced at lower temperatures because the magnetostrictive strain takes the system away from quantum criticality. The results at low temperatures are in strong contrast to those obtained from those obtained from a perturbation theory in which the Landau parameter B is reduced as this gives a much larger value of the magnetization at low temperatures as was seen in Figs. 2(a) and 2(b). This difference would also apply to any other mechanism for obtaining a QCP which resulted in an enhanced, but constant, value of B.

These plots include the result from the linear theory where the effects of the dependence of the transition temperature on strain are approximated by a term that is linear in $(\varepsilon - \varepsilon_s)$, which has the effect of changing the Landau parameter from B to B' is shown as is the result labeled linear theory, for completeness we show the plot where T_c has been reduced but the value of B is unchanged. The magnetization is shown for various pressures in Fig. 5.

In these figures, the temperature is defined in units of the transition temperature of the unstrained material. Close to a QCP, at ε_o, the rapid dependence of the strain on the magnetization means that the linearized theory is only a good approximation very close to the phase transition in the second order regime
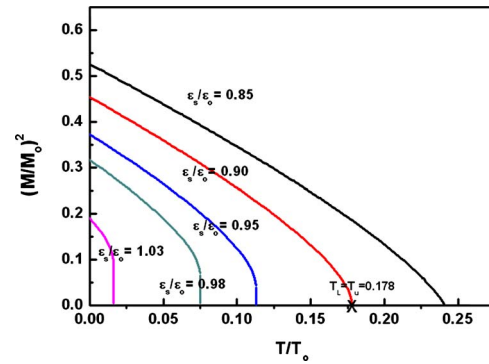
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