First-Order Superconducting Transition near a Ferromagnetic Quantum Critical Point

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We address the issue of how triplet superconductivity emerges in an electronic system near a ferromagnetic quantum critical point (FQCP). Previous studies found that the superconducting transition is of second order, and T_c is strongly reduced near the FQCP due to pair-breaking effects from thermal spin fluctuations. In contrast, we demonstrate that near the FQCP, the system avoids pair-breaking effects by undergoing a *first order* transition at a much larger T_c. A second order superconducting transition emerges only at some distance from the FQCP.

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Superconductivity near a magnetic instability is a topic of current interest in condensed-matter physics. Magnetically mediated pairing near an antiferromagnetic instability is a candidate scenario for d-wave superconductivity in the cuprates and heavy fermions compounds (for a recent review, see [1]). Superconductivity mediated by the exchange of ferromagnetic spin fluctuations is also expected near ferromagnetic transitions. Ferromagnetic exchange yields Cooper pairs with $S = 1$ and, therefore, generally gives rise to triplet pairing originally suggested for ^{3}He (Ref. [2]). In recent years, an intensive search has focused on superconductivity in compounds which can be tuned to a ferromagnetic quantum critical point (FQCP) by varying either pressure or chemical composition. Examples include MnSi and the heavy fermion compound UGe_2 (for an experimental review, see Ref. [3]).

The emergence of superconductivity in electronic systems close to a ferromagnetic instability has recently been studied by three groups, who solved a linearized gap equation within the Eliashberg formalism [4–6]. In both two- (2D) and three-dimensional (3D) systems, their analysis yielded a superconducting transition temperature T_c^l (l stands for linearized) that substantially decreases as the system approaches criticality.

The physical origin of the decrease in T_c^l near the FQCP lies in the presence of thermal spin fluctuations which behave like magnetic impurities whose scattering potential diverges as the critical point is approached [4–6]. This behavior is reflected in the fermionic self-energy in the normal state, $\Sigma(\omega_n) \propto iT\sum_m \text{sgn}(\omega_n)\chi_L(\omega_m - \omega_n)$, where $\chi_L(\omega) = \int d^{D-1}q\chi(q, \omega)$ is the "local" spin susceptibility. Since $\chi_L(\omega = 0)$ diverges at the FQCP for $D \leq 3$ [assuming $\chi(q, 0) = \chi_0/(\xi^{-2} + q^2)$ with $\xi \to \infty$], the dominant contribution to $\Sigma(\omega_n)$ comes from the $n = m$ term in the frequency sum, i.e., from classical, thermal spin fluctuations. These fluctuations scatter with a finite momentum and zero frequency transfer, hence their similarity to magnetic impurities. This leads to $\Sigma(\omega) = i\gamma\text{sgn}\,\omega$ with $\gamma \propto T\xi^{3-D}$ for system dimension $D < 3$ and $\gamma \propto T\log\xi$ for $D = 3$.

The analogy with magnetic impurities extends to the pairing problem in which thermal spin fluctuations close to the FQCP tend to break Cooper pairs and hence lower the temperature of the superconducting transition [7]. Simple estimates show that the linearized gap equation does not have a solution above $\gamma \sim T_{c0}$, where T_{c0} is the transition temperature in the absence of thermal fluctuations. Hence, near FQCP, T_c^l vanishes as $T_c^l \propto \xi^{D-3}$ in $D < 3$ and $T_c^l \propto 1/\log\xi$ for $D = 3$. Numerical solutions of the linearized Eliashberg equations near a ferromagnetic instability demonstrate precisely this kind of behavior—T_c^l falls off when the FQCP is approached—more rapidly in 2D [4] than in 3D [5,6].

In this Letter, we argue that the actual behavior of the system is different from that discussed in Refs. [4–6]. We show that close to a FQCP, superconductivity emerges via a *first order phase transition* at $T_c \sim T_{c0}$. The much smaller T_c^l previously obtained by solving the linearized gap equation is just the end point of the temperature hysteresis loop at which the normal state becomes unstable. We argue that the first order transition originates in the fact that the feedback effects from the pairing on ferromagnetic spin fluctuations give rise to a smooth evolution of the pairing gap from $T = 0$ when dangerous thermal effects are absent and Δ is large, up to $T \sim T_{c0}$.

The physics that leads to first order transition can be understood by considering the ratio of the divergent terms in the self-energy and the pairing vertex. These terms appear with different signs in the gap equation; hence, if the overall factors were the same, the pair-breaking effects would be canceled out as happens in a dirty s-wave superconductor with nonmagnetic impurities. In our case, the overall factors are not equal as $\Sigma_{\alpha\beta} = \Sigma\delta_{\alpha\beta}$, and the spin factor in the self-energy diagram is 3 as $\sum_\gamma \boldsymbol{\sigma}_{\alpha\gamma}\boldsymbol{\sigma}_{\gamma\beta} = 3\delta_{\alpha\beta}$. Meanwhile, the triplet pairing vertex $\Gamma_{\alpha\beta} = \Gamma\delta_{\alpha\beta}$, and the spin factor in the vertex renormalization diagram is 1 as $\sum_{\gamma,\delta}\delta_{\gamma\delta}\boldsymbol{\sigma}_{\gamma\alpha}\boldsymbol{\sigma}_{\delta\beta} = \delta_{\alpha\beta}$.

The ratio of the divergent terms in the self-energy and in the pairing vertex is then 3:1; i.e., the pair-breaking effects are not canceled out, and T_c^l vanishes at criticality. The fact that a pair has $S = 1$ is crucial here as in the case of singlet pairing (mediated by, e.g., antiferromagnetic spin fluctuations), $\Gamma_{\alpha\beta} = \Gamma\sigma^y_{\alpha\beta}$, and the spin summation for the pairing vertex yields (with the extra overall minus sign due to d-wave pairing) $\sum_{\gamma,\delta}(-1)\sigma^y_{\gamma\delta}\boldsymbol{\sigma}_{\gamma\alpha}\boldsymbol{\sigma}_{\delta\beta} = 3\sigma^y_{\alpha\beta}$, i.e., the divergent terms cancel each other, and T_c^l saturates at a finite value for $\xi = \infty$ [8].

Consider next a triplet superconducting state, which can be of either the A or the B type [2,9]. Since the low-energy fermions acquire a gap, the low-energy part of the spin susceptibility, arising from these fermions, changes. In the A phase, we can assume without loss of generality that the spin of the Cooper pair $\vec{S}_{\rm cp}$ lies in the xy plane in spin space. Obviously, the feedback effects on the spin susceptibility are then different for χ_{zz} and $\chi_\pm$. When $\chi_\pm$ and χ_{zz} are not equivalent, the spin summation shows that the former 3:1 ratio of the dangerous terms becomes $[2\chi_\pm + \chi_{zz}]/[2\chi_\pm - \chi_{zz}]$. We show that in the superconducting state, $\chi_\pm$ remains massless at the FQCP, but χ_{zz} acquires a mass and becomes nondivergent. Then the divergent terms from the fermionic self-energy and the pairing vertex cancel out in the *nonlinear* gap equation. This implies that the superconducting state remains stable well above T_c^l, but only as long as $\Delta(\omega)$ is not small; otherwise, $\chi^L_{zz}(0)$ cannot be neglected, the above ratio of divergent terms again becomes 3, and no cancellation occurs. Thus, we expect that at the FQCP, the solution with a finite gap survives up to the end point at $T_c^{\rm nl} \sim T_{c0} \gg T_c^l$ (nl stands for the solution of the nonlinear equation) where it becomes unstable. This is a classic first order transition.

In the B phase, the situation is simpler: the thermal spin susceptibility remains isotropic, but all of its components become massive and do not diverge in a superconductor [9]. This again implies that the large gapped superconducting state remains stable well above T_c^l, but only as long as the gap remains large.

In the remainder of this Letter we consider the A phase and compute $T_c^{\rm nl}$ from the full set of nonlinear Eliashberg equations. Our starting point is the spin-fermion model, which describes the interaction of low-energy fermions with their own spin degrees of freedom, $\mathbf{S_q}$, whose propagator is peaked at $q = 0$. The same model was used in earlier studies [4–6,8,10]. We assume that T_{c0} is much less than the Fermi energy E_F, implying that the pairing instability involves only fermions near the Fermi surface. The model is described by the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k},\alpha} \mathbf{v_F}(\mathbf{k} - \mathbf{k}_F)c^\dagger_{\mathbf{k},\alpha}c_{\mathbf{k},\alpha} + \sum_q \chi^{-1}(\mathbf{q})\mathbf{S_q}\mathbf{S_{-q}} + g\sum_{\mathbf{q},\mathbf{k},\alpha,\beta} c^\dagger_{\mathbf{k+q},\alpha}\boldsymbol{\sigma}_{\alpha,\beta}c_{\mathbf{k},\beta}\cdot\mathbf{S_{-q}}. \quad (1)$$

where the spin-fermion coupling, g, the Fermi velocity, v_F (we assume a circular Fermi surface), and the static spin propagator $\chi(q,0)$ are input parameters. The dynamical part of $\chi(q,\Omega_m) = \chi_0/[q^2 + \xi^{-2} + \Pi(q,\Omega_m)]$ arises from the interaction with the low-energy fermions and is explicitly calculated. While we restrict our consideration to $D = 2$, our conclusions are also valid for 3D systems.

We assume that the static $\chi(q,0)$ has the conventional Lorentzian form with a weakly temperature dependent ξ. This form of $\chi(q,0)$ was recently questioned [11,12] since far away from criticality, the static spin susceptibility possesses singular low-energy *Fermi liquid* corrections that give rise to a universal $|q|$ dependence of $\chi(q,0)$ and a T dependence of ξ^{-1}. As it is unclear whether these singular corrections survive in the quantum-critical regime, we restrict to the conventional form of $\chi(q,0)$.

Near the critical point, a conventional perturbation theory in the spin-fermion coupling (for which $\Sigma = \Pi = 0$ is the point of departure) holds in powers of $\lambda = g^2\chi_0/(4\pi v_F\xi^{-1})$, i.e., the quantum-critical region falls into the strong coupling limit. An approach for dealing with a strong coupling problem is the Eliashberg theory [13]. Its validity requires certain restrictions that we discuss after presenting the results.

We first consider the situation right at the FQCP. In the normal state, the dynamical part of the spin polarization operator, $\Pi(q,\Omega_m)$, is independent of the fermionic self-energy, $\Sigma(q,\omega_n)$ (but not vice versa), as the essential momenta for $\Pi(q,\Omega_m)$ are those with $v_Fq \gg \Omega_m, \Sigma$. As a result, $\Pi(q,\Omega_m)$ has the same form as for free fermions, i.e., for $|\Omega_m| \ll v_Fq$, $\Pi(q,\Omega_m) = F(\Omega_m)/(v_Fq)$ where $F(\Omega_m) = \alpha k_F^2|\Omega_m|$, $\alpha = g^2\chi_0/(2\pi E_F)$, and $E_F = k_Fv_F/2$. At the same time, $\Sigma(\omega)$ is determined by Π and given by $\Sigma(\omega_m) = \omega_0^{1/3}\omega_m^{2/3}$, where $\omega_0 = (3\sqrt{3}/4)\alpha^2E_F$. The non-Fermi liquid, $\omega^{2/3}$ dependence of the self-energy in 2D is due to the divergence of the perturbation theory at the FQCP. This form was earlier obtained in Ref. [14].

In the superconducting state, the equations for two components of $F(\Omega)$ (F_{zz} and $F_{xx} = F_{yy}$) are coupled to the equation for the pairing gap $\Delta(\omega)$. Thus, one must self-consistently solve a set of three coupled equations for the two components of F and Δ. The derivation of the Eliashberg equations is straightforward and will not be presented here. The Cooper pair spin lies in the xy plane, and the coupled equations for $\Delta(\omega)$, $F_{zz}(\Omega) = F_-$, and $F_{xx} = F_{yy} = F_+$ at the FQCP are

$$\Delta(\omega_n) = T\sum_m \frac{4\pi\omega_0^{1/3}/9}{\sqrt{\omega_m^2 + \Delta^2(\omega_m)}}\left\{\frac{2\omega_m}{[F_+(T,\Delta,\omega_m-\omega_n)]^{1/3}}\left[\frac{\Delta(\omega_m)}{\omega_m} - \frac{\Delta(\omega_n)}{\omega_n}\right] - \frac{\omega_m}{[F_-(T,\Delta,\omega_m-\omega_n)]^{1/3}}\left[\frac{\Delta(\omega_m)}{\omega_m} + \frac{\Delta(\omega_n)}{\omega_n}\right]\right\} \quad (2)$$

and

$$F_{\pm} = \pi T \sum_n \left[1 - \frac{\omega_n \omega_m \pm \Delta(\omega_n)\Delta(\omega_m)}{\sqrt{\omega_n^2 + \Delta^2(\omega_n)}\sqrt{\omega_m^2 + \Delta^2(\omega_m)}} \right]. \quad (3)$$

As anticipated, $F_+(T, \Delta, 0) = 0$ vanishes, implying that the corresponding susceptibilities, χ_{xx} and χ_{yy}, describe massless modes. The vanishing of $F_+(T, \Delta, 0)$, however, is not dangerous as it is compensated by the simultaneous vanishing of the numerator in Eq. (2). Exactly the same cancellation of divergences occurs in the gap equation for d-wave pairing due to antiferromagnetic spin fluctuations. The vanishing of $F_-(T, \Delta, 0)$ would be dangerous, but for finite Δ, $F_-(T, \Delta, 0) = 2\pi T \sum_n \Delta^2(\omega_n)/\sqrt{\omega_n^2 + \Delta^2(\omega_n)}$ is also finite, i.e., the longitudinal spin excitation described by $\chi_{zz}^{-1}(\omega = 0) \propto q^2 + F_-(T, \Delta, 0)/(v_F q)$ is massive. In contrast, for the linearized gap equation Δ is vanishingly small, $F_-(T, \Delta, 0)$ vanishes, and the right-hand side of Eq. (2) diverges. Because of this divergence, the linearized gap equation does not have a solution down to $T = 0$. Note that the only energy scale in the Eliashberg equations is ω_0, which can be eliminated by rescaling both temperature and the gap in units of ω_0. The gap equation is then *fully universal*, which implies that the mass in χ_{zz} and the typical momentum q for the pairing problem are both of order ω_0/v_F.

In Fig. 1(a) we present the numerical solution for $\Delta(T)$ at the lowest Matsubara frequency, $\omega_m = \pi T$. As expected for a first order phase transition, the gap changes discontinuously from a finite value to zero at $T_c^{\rm nl} \sim 0.015\omega_0$. The inset shows that the discontinuous jump in Δ occurs for all Matsubara frequencies. In addition to the two stable solutions for $\Delta(\omega)$ that we found, there also exists an unstable one corresponding to a maximum of the free energy. We did not study this extra solution and focused only on the stable one, which continuously evolves from the only solution for the gap at $T = 0$.

We next study the situation at finite ξ and verify whether the first order superconducting transition becomes second order at some distance from the FQCP. Away from criticality, the equations for $F_{\pm}(T, \Delta, \omega_m)$ retain their form, but in the gap equation, the factors $F_{\pm}(T, \Delta, \omega_m)$ are replaced by $F_{\pm}(T, \Delta, \omega_m)/I^3(\beta_{\pm})$, where $I(\beta_{\pm})$ by itself depends on $F_{\pm}(T, \Delta, \omega_m)$ through

$$I(\beta_{\pm}) = \frac{3\sqrt{3}}{2\pi} \int_0^{\infty} dx \frac{x}{1 + \beta_{\pm} x + x^3}, \quad (4)$$

$\beta_{\pm} = b/[F_{\pm}(T, \Delta, \Omega_m)/\omega_0]^{2/3}$, and $b = (8/3\sqrt{3})^{2/3} \times (\alpha k_F \xi)^{-2}$ measures the deviation from the FQCP ($b = 0$ at the FQCP). At finite ξ, the gap equation contains no divergences, even at infinitesimally small Δ; thus, both $T_c^{\rm nl}$ and T_c^l are nonzero.

In Fig. 1(b) we plot $\Delta(T, i\pi T)$ for $b = 2$. We see that the temperature dependence of the gap is now continuous, in marked distinction to Fig. 1(a). The inset shows that the continuous evolution of Δ holds for all Matsubara frequencies. This implies that for large enough $b > b_c$, the transition is second order. To locate the tricritical point $b = b_c$, we plot in Fig. 1(c) the magnitude of the jump of $\Delta(T, i\pi T)$ at $T_c^{\rm nl}$ as a function of b. The gap discontinuity disappears at $b_c \approx 1.2$. For completeness, in Fig. 1(d) we plot the zero temperature gap versus b. We see that it changes gradually, without a singularity at b_c.

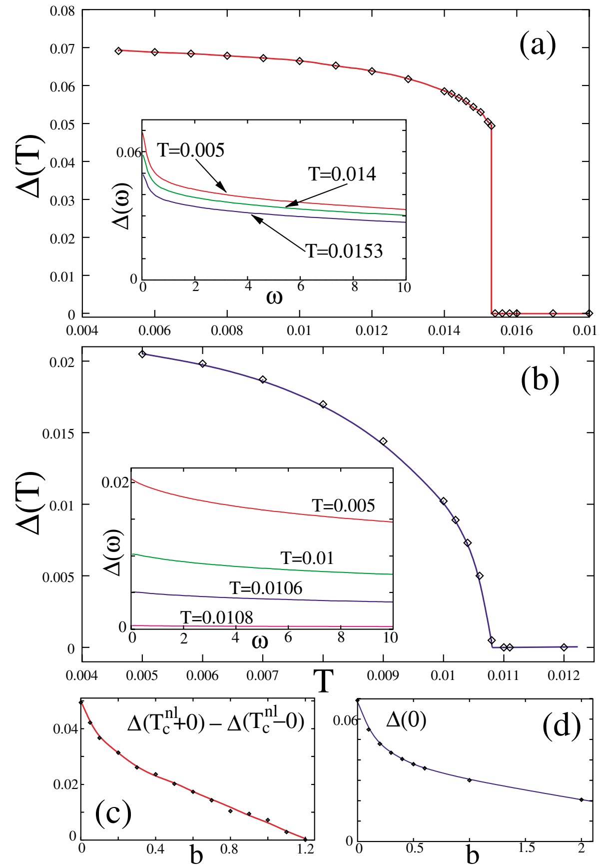

FIG. 1 (color online). (a) Temperature dependence of $\Delta(T, \omega_m)$ at the lowest Matsubara frequency $\omega_m = \pi T$ for $b = 0$. The lines are a guide for the eye. Δ, T and ω_m are in units of ω_0 (see text). The discontinuity of $\Delta(T)$ at 0.015 indicates a first order transition. The inset shows $\Delta(\omega)$ versus frequency at several T. (b) Same away from the FQCP, for $b = 2$. Now the transition is continuous. (c) The magnitude of the jump of $\Delta(T, i\pi T)$ at the instability temperature versus b. The line is a guide to the eye. (d) $\Delta(T, i\pi T))$ at the lowest T versus b.

We present the phase diagram in Fig. 2. Our $T_c^l(b)$ agrees with earlier results [4–6]. The actual superconducting transition temperature, however, lies between T_c^l and $T_c^{\rm nl}$ and remains *finite* at $b = 0$. For $0.9 \lesssim b < b_c$, the jump in Δ at $T_c^{\rm nl}$ and consequently the difference between T_c^l and $T_c^{\rm nl}$ is small but finite [see Fig. 1(c)]. The inset shows the reduction of T_c at large b due to the decreased effective coupling.

Finally, the validity of the Eliashberg treatment requires that three conditions be satisfied. First, typical bosonic momenta q_B should be much larger than typical fermionic $|k - k_F|$, i.e., bosons should be slow modes

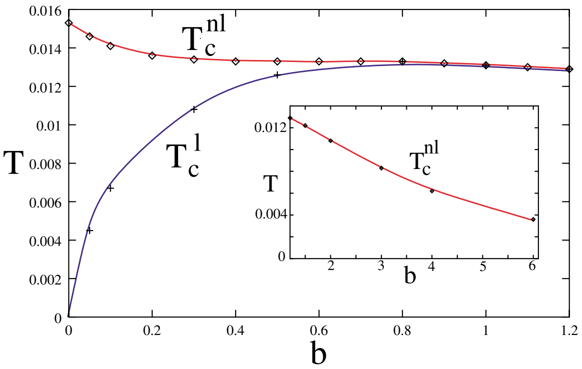

FIG. 2 (color online). The phase diagram near the FQCP. In the near vicinity of the FQCP, the transition is of first order, away from the FQCP; to the right of b_c, it is of second order. For the first order transition, $T_c^{\rm nl}$ and T_c^l are the instability temperatures for the solutions with a large and infinitesimally small gap, respectively. The actual first order transition temperature, T_c, lies between T_c^l and $T_c^{\rm nl}$. Inset: the reduction of T_c at large b.

compared to fermions, leading to $\Sigma(k, \omega) \approx \Sigma(\omega)$. A straightforward analysis shows that the typical $q_B \sim \alpha k_F$, while the typical $|k - k_F| \sim \omega_0/v_F \sim \alpha^2 k_F$. The Eliashberg theory is therefore valid if $\alpha \ll 1$, i.e., $\omega_0 \ll E_F$. This in turn implies that the physical behavior of the system is universally determined by only low-energy excitations. Second, vertex corrections should be small. Generally, this is not possible for typical $q_B \ll k_F$, as vertex corrections scale with ξ. However, for $\alpha \ll 1$, we require only the vertex for $\Omega \ll v_F q$ since the typical $v_F q_B$ well exceeds the typical $\Omega \sim \omega_0$. In this limit, vertex corrections are much smaller and only scale as $\log\xi$. They are still non-negligible at the FQCP, where they change the pole in the spin susceptibility into a branch cut [10]. However, we verified that, as in the antiferromagnetic case [8], this only leads to a small renormalization of the prefactors in the gap equation. Third, one should be able to neglect the momentum dependence of the pairing gap, while preserving the gap symmetry, $\Delta(\vec{n} k_F) = -\Delta(-\vec{n} k_F)$. This approximation is again justified by $\alpha \ll 1$, as in this limit, the typical momentum transfers along the Fermi surface $\delta k \sim q_B \sim \alpha k_F$ are much smaller than k_F. In this situation, the momentum variation of the gap at typical δk introduces only $O(1)$ corrections to the Eliashberg theory [8], which can be safely neglected. Note in passing that the smallness of $\delta k \ll k_F$ makes our theory also applicable to real materials (in which a crystalline structure imposes additional constraints on the order parameter symmetry [15]), as it allows one to consider the pairing problem in a local-momentum approximation, ignoring the peculiarities of the gap's momentum dependence.

In summary, we showed that near a FQCP, spin fluctuation exchange gives rise to a strong first order transition into a triplet superconducting state. By choosing a first order transition, the system avoids divergent pair-breaking effects from thermal spin fluctuations. As a result, T_c saturates at a nonzero value at criticality. The first order transition persists up to a finite distance from the FQCP, where it becomes second order.

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