Local Defect in Metallic Quantum Critical Systems

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(Received 13 April 2001; published 1 October 2001)

We present a theory of a single point, line, or plane defect coupling to the square of the order parameter in a metallic system near a quantum critical point at or above its upper critical dimension. At criticality, a spin droplet is nucleated around the defect with its core size determined by the strength of the defect potential. Outside the core a universal slowly decaying tail of the droplet is found, leading to many dissipative channels coupling to the droplet and to a complete suppression of quantum tunneling. We propose an NMR experiment to measure the impurity-induced changes in the local spin susceptibility.

DOI: 10.1103/PhysRevLett.87.167202 PACS numbers: 75.10.Jm, 75.10.Nr, 75.70.Kw, 76.30.Da

The behavior of "droplets" of local order in a nonordered background is an issue of wide relevance in condensed matter physics. One particularly interesting subclass of problems concerns droplets induced by defects in nearly critical systems. A long-standing problem in heavy fermion physics concerns the very small magnetic moments which have been observed in several materials [1,2] and may be related to grain boundaries and other structural defects [3,4]. In a colossal magnetoresistance material, magnetic order was observed to be enhanced near grain boundaries [5]. A related issue is the magnetism induced in high temperature superconductors by apparently nonmagnetic substituents such as Zn [6], which have been interpreted [7,8] as spin droplets induced in a nearly critical system (although other interpretations also exist [9]). Nucleation of regions of charge density wave order around defect sites on the surface of a "correlated" material was reported by [10]. "Quantum Griffiths" effects and "Kondo disorder" are presently of intense interest [11–14]. The problem bears on the fundamental issue of the Kondo effect near a quantum critical point [15]. Finally, recording of information involves the polarization of small domains, whose long time dynamics and stability are of great importance.

This Letter presents the theory of the local polarization ("droplet") induced by a single defect in an otherwise nondisordered system which is near a quantum critical point at or above its upper critical dimension, d_u. These restrictions allow a controlled theoretical treatment and apply to a wide range of systems including metallic magnets in dimensions $d = 2, 3$ [16,17] and "quantum paraelectric" (i.e., nearly ferroelectric) systems in $d = 3$ [18]. We study defects which couple to the square of the order parameter, i.e., change the "local T_c," and thus may create small regions (droplets) where the order parameter is nonvanishing at least on short time scales. We address three questions: Under which circumstances does the defect create a droplet? What is the size and other properties of the droplet? What are the relevant fluctuations? Our work is complementary to that of Vojta and Sachdev [19], who studied a linear coupling of the defect to the order parameter in a quantum critical system below d_u, and differs in several aspects from the related work of Castro-Neto and Jones [12,13].

Our starting point is a quantum Ginzburg-Landau action for an order parameter field ϕ. Halperin and Varma used a similar approach for a classical system [20]. After obtaining the mean-field solution we consider fluctuation corrections, which are tractable because the dimension of the system is above d_u. Our action, in conveniently scaled variables, is $S = S_{\text{stat}} + S_{\text{dyn}}$ with

$$S_{\text{stat}} = \frac{1}{2}\int_0^{E_0/T} d\tau \int d^d x \times \left\{ (V(\mathbf{x}) + \kappa^2)\phi(\mathbf{x},\tau)^2 + [\nabla\phi(\mathbf{x},\tau)]^2 + \frac{1}{2}\phi(\mathbf{x},\tau)^4 \right\}. \quad (1)$$

Here, κ determines the distance of the bulk system to the critical point. We measure lengths in units of the bare correlation length ξ_0 of the problem (typically of the order of a lattice constant) and measure energies in terms of the condensation energy E_0 obtained by evaluating the static, spatially uniform free energy with $\kappa = 1$. In the following, we consider only symmetrical defects, which are characterized by a dimensionality d_d (i.e., the number of dimensions along which the defect potential, V, remains constant), a length scale a (expected to be $\lesssim\xi_0$) over which V decays in the $D = d - d_d$ transverse directions, and a dimensionless strength $v = -\int d^D r\, V(\mathbf{r})$ ($v > 0$ corresponds to a local tendency towards order). Here, $\mathbf{r}$ refers to the $D = d - d_d$ transverse components of the d-dimensional vector $\mathbf{x}$, where $d_d = 0, 1, 2$ corresponds to a point, line, and plane defect, respectively.

The dynamic term S_{dyn} takes the general form

$$S_{\text{dyn}} = \frac{T}{2}\sum_{\mathbf{q},\omega_n}\left(\frac{1}{c_{\mathbf{q}}^2} + \frac{1}{\Gamma_{\mathbf{q}}|\omega_n|}\right)|\omega_n\phi(\mathbf{q},\omega_n)|^2. \quad (2)$$

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where the coefficients c and Γ depend on whether the system is overdamped (metallic case) or not, on the symmetry of the order parameter, and on whether it is conserved. Examples include (i) the undamped Ising antiferromagnet, with $\Gamma^{-1} = 0$ and $c = \text{const}$; (ii) the undamped Ising ferromagnet with a conserved order parameter, $\Gamma^{-1} = 0$ and $c \sim 1/q$; (iii) the metallic (overdamped) antiferromagnet [16,17] $\Gamma = \text{const}$; (iv) the metallic Ising ferromagnet $\Gamma_{\mathbf{q}} \sim q$. The form of S_{dyn} combined with the static part of the free energy defines a (mean-field) dynamic exponent z which is $z = 1, 2, 2, 3$ respectively, for the cases listed above. The effective dimensionality of the quantum phase transition problem defined by S is $d_{\text{eff}} = d + z$ and we restrict it to $d_{\text{eff}} \geq 4$. These expressions assume that the droplet is small enough that all relevant bulk electronic states may penetrate it; we show below that this assumption is correct for the droplets we consider.

We now sketch the essential features of the mean-field solution (details will be given elsewhere [21]). We focus only on the transverse dimensions and assume $V(r > a) = 0$ so that for $r > a$ the mean-field equation is

$$-\nabla^2\phi_0 + \kappa^2\phi_0 + \phi_0^3 = 0\,. \tag{3}$$

For $0 \leq \kappa \ll 1$, the solution is of the form $\phi_0(r) = r_0^{-1} f(r/r_0, \kappa r_0)$, where f is dimensionless. The length scale r_0 is determined by connecting the solution of Eq. (3) (i.e., for $r > a$) to the solution for $r < a$ and thus depends on the defect strength, v. For $\kappa r_0 > 1$ the ϕ^3 term may be neglected at all r and the solution is the familiar exponentially decaying solution. For $\kappa r_0 < 1$ and $D \leq 3$, the behavior at $r < \kappa^{-1}$ is controlled by the nonlinearity and the scale r_0 defines the size of the droplet. The results are summarized in Table I.

In $D = 1, 2$, and in $D = 3$ up to logarithms, the $r_0 < r < \kappa^{-1}$ behavior of $\phi_0(r)$ is independent of the short length scale physics encoded in r_0. In all dimensions, $\int d^D r\, \phi_0(r)$ diverges at criticality and, in $D \geq 2$, $\int d^D r\, \phi_0^2(r)$ diverges. Thus many physical properties are dominated by the $r > r_0$ "tail" of $\phi_0(r)$. Figure 1a shows a schematic picture of the droplet amplitude.

The scale r_0 may be estimated by substituting our results for $\phi_0(r)$ into Eq. (1) and minimizing with respect to r_0. This also determines the binding energy, E_{bind}, of the droplet which forms at temperatures $T < E_{\text{bind}}$. Alternative approaches including scaling, exact solutions ($D = 1$), and numerics give identical results [21]. In all cases the energetics are dominated by the droplet "core" region $r < r_0$. At criticality, an arbitrarily weak potential induces a droplet in $D = 1, 2$ but in $D = 3$ a critical strength is required. In $D = 1$, $r_0 \sim v^{-1}$ and $E_{\text{bind}} \sim -E_0 v^3$ while, in $D = 2$, $r_0 \sim e^{1/v}$ and $E_{\text{bind}} \sim -E_0 v e^{-2/v}$. In $D = 3$, a critical value $v^* \sim 1$ is required for droplet formation, and, for $v > v^*$, r_0 is of order a while $E_{\text{bind}} \sim -E_0 \frac{v}{v^*}(\frac{v}{v^*} - 1)a^{-2}$. The droplet size cannot exceed κ^{-1}, which yields an estimate for the critical potential $v^*(\kappa) = 2\kappa$ ($D = 1$) and $v^*(\kappa) = -2\pi/\log(\kappa a)$ ($D = 2$). The droplet magnetization M_d in the ferromagnetic case is given by the integral of $\phi_0(\mathbf{r})$ which diverges as κ^{1-D} (logarithmically in $D = 1$) as criticality is approached. In an antiferromagnetic system with characteristic wave vector $\mathbf{Q}$, $M_d \sim |\mathbf{Q}|^{1-D}$ which for $D \geq 1$ is a number of order unity even at criticality. The droplet potential opens a local gap in the bulk electronic spectrum. The penetration of these gapped states into the droplet is controlled by the length scale $L(r) \sim v_F\xi_0/E_0\phi_0(r)$. In $D = 3$ our result for ϕ gives $L(r)/r \sim \ln(r_0/r)^{1/2} > 1$ so the properties (especially dissipation) are bulklike everywhere. In $D = 1, 2$ we have $L(r_0)/r_0 = v_F\xi_0/E_0$, where typically $v_F\xi_0/E_0 \gtrsim 1$, again implying bulklike dissipation. However, for $v_F\xi_0/E_0 \ll 1$ a modification of the dissipation term is required [21].

Gaussian fluctuations may be treated by expanding to quadratic order about the mean-field solution, leading to the action,

$$S_{\text{GF}} = S_{\text{dyn}} + \frac{T}{2}\int d^d x \sum_{i\omega_n} \psi(\mathbf{x}, \omega_n)\hat{L}\psi(\mathbf{x}, \omega_n)\,, \tag{4}$$

TABLE I. Approximate behavior of a droplet wave function in different length (r) regimes and relative dimensionalities (D). The g_D are constants; r_0, κ are defined in the main text.

D	$r < r_0$	$r_0 < r < \kappa^{-1}$	$\kappa^{-1} < r$
1	$g_1 r_0^{-1}$	$\sqrt{2}/r$	$\sqrt{2}\,\kappa e^{-\kappa r}$
2	$\frac{g_2 \ln(\frac{r}{r_0}) + g_2'}{r_0}$	$1/r$	$e^{-\kappa r}/r^{1/2}$
3	g_3	$\ln^{-1/2}(\frac{r_0}{r})/r$	$e^{-\kappa r}\ln^{-1/2}(\kappa r_0)/r$
>3	$g_D r_0$	r_0^{D-3}/r^{D-2}	$e^{-\kappa r} r^{(1-D)/2}$

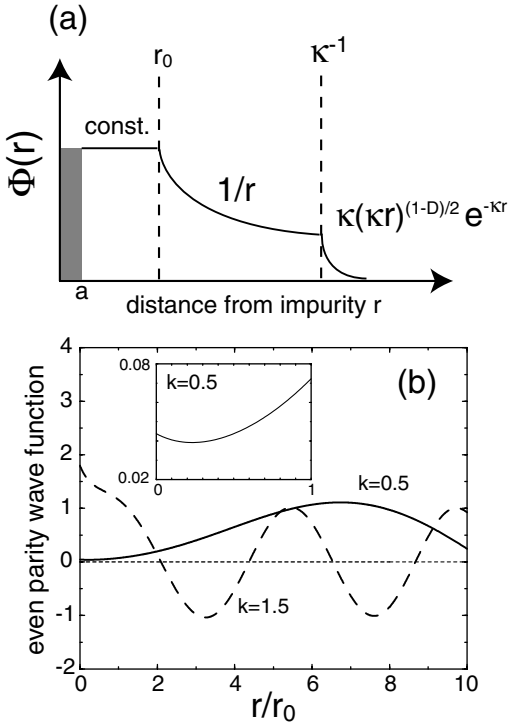

FIG. 1. (a) Schematic r dependence of the droplet amplitude, $\phi_0(r)$. (b) Dependence of even parity wave functions for $k = 0.5$ and $k = 1.5$ on the distance from the defect. Inset: near-defect ($r \approx r_0$) region for $k = 0.5$.

where $\hat{L} = \kappa^2 + V(\mathbf{x}) + 3\phi_0^2(\mathbf{x}) - \nabla_{\mathbf{x}}^2$. $\hat{L}$ has only positive energy eigenfunctions. At criticality all of these are extended, but if $\kappa \neq 0$ then, for v in a small range above v^*, a bound state of energy $0 < E < \kappa^2$ may occur. The form of the potential (weak slowly varying repulsion with an attractive center) leads to nonmonotonic wave functions with an upwards cusp at the defect scale a, a decrease with distance in the range between a and r_0, and then (for extended states) an increase back to the unit amplitude of a propagating plane wave. This is shown for two even parity wave functions in Fig. 1b. The effect of Gaussian fluctuations on the droplet size and shape may be computed in terms of the difference between the eigenfunctions of $\hat{L}$ and of $\kappa^2 - \nabla^2$ and is found [21] not to change the long distance behavior of the droplet.

A more important class of fluctuations changes the orientation of the droplet. In a compact ($d_d = 0$) droplet these are rotations and "instanton" processes in which the droplet collapses and reforms. In extended ($d_d > 0$) droplets the important processes are motions of domain walls. Here, we sketch the results for a compact droplet; details and an analysis of the moving domain wall case will be given elsewhere [21]. The dynamics of an isolated (not embedded in a critical system) droplet have been previously studied [22]; the new feature here is the overdamped dynamics (in the metallic case).

We first consider a droplet with Ising symmetry, in which case the instanton, i.e., the collapse of the droplet, is the important fluctuation process. To estimate the action we substitute the ansatz $\phi(\mathbf{r}, \tau) = \phi_0(\mathbf{r})\eta(\tau)$ into Eq. (1) and retain leading time derivatives. We find that the action corresponding to $2N$ instantons is

$$S_{2N} = \frac{\gamma}{2} \sum_{i \neq j = 1,\ldots,N} \log(y_i - y_j)(-1)^{i+j} + 2NS_0, \quad (5)$$

with the single-instanton action S_0 given by $S_0 = (\frac{y_0}{\zeta} + \frac{m}{y_0}) + \frac{2N\gamma}{4} \int_{-1}^{1} du \int_{-1}^{1} dv \log[1 + y_0^2(u - v)^2]$, $\zeta = 15E_0/(4E_{\text{bind}})$, $m = E_0^2 \sum_{\mathbf{q}} c_{\mathbf{q}}^{-2} \phi_0(\mathbf{q})^2$, and $\gamma = E_0 \sum_{\mathbf{q}} \Gamma_{\mathbf{q}}^{-1} \phi_0(\mathbf{q})^2$. The quantity y_0 is the duration of an instanton in units of E_{bind}^{-1} and is found by minimizing S_0. Note that both m and γ diverge as $\kappa \to 0$ and that $\gamma = 0$ in undamped models. In the weak dissipation ($\gamma \ll 1$) limit the standard macroscopic quantum tunneling analysis [23] leads to $S(y_0) = 8\sqrt{m/\zeta} + 6m\gamma\zeta + \mathcal{O}(\gamma^2)$ so that the "bare" droplet tunneling rate is $\sim E_0 e^{-S(y_0)}$ and vanishes as criticality is approached. Instanton-instanton interaction effects, which arise from the first term in S_{2N}, are handled via a perturbative renormalization group treatment, and, if γ is less than a critical value ~ 1, dissipative effects reduce the tunneling rate but not to zero.

In a metallic system near criticality, $\gamma \gg 1$, and the conventional analysis does not apply. Our detailed results depend on the ratio m/γ. If $m/\gamma \gg 1$ (ferromagnetic case) then minimization leads to $S(y_0) = 2\gamma[\log(m/2\gamma) + 1]$ while for $m/\gamma \ll 1$ we find $S(y_0) = 3m(\gamma/6m)^{1/3}$. In either case, dissipation strongly suppresses the bare tunneling rate, and the large value of γ puts the action on the localized side of the Caldeira-Leggett phase boundary, implying that tunneling processes are completely suppressed on long time scales.

Our treatment closely parallels Hamann's formulation [24] of the Kondo dynamics of a single spin in a noncritical metal. Hamann found $S(y_0) = \ln(1/JN_0)$ (J is the Kondo coupling and N_0 is the Fermi surface density of states) and $\gamma = (1 - JN_0)^2$. The crucial difference is that in our problem the large size of the droplet allows many dissipative channels to couple to it, leading to much stronger dissipative effects. Castro-Neto and Jones [12] argued that the tunneling of a droplet could be mapped onto a single-channel Kondo problem; in our model this is not the case. A subsequent paper [13] considered a droplet consisting of a large number of elementary $S = 1/2$ spins in $d = 3$ locked together by some magnetic interaction in a nearly critical system. They neglected the $1/r$ tail of the droplet so their specific results differ from ours. They found that, for antiferromagnetic systems, droplets as large as 10^3 spins could tunnel and that dissipative effects only became important below an exponentially small scale, leaving a wide regime where quantum Griffiths behavior might occur, whereas we find that near criticality dissipation always dominates.

In droplets with XY or higher symmetry, rotational fluctuations must be considered. We begin from an action of the type discussed in [25] and assume that ϕ is characterized by an amplitude $\phi_0(\mathbf{r})$, obtained by solving Eq. (3), and a direction $\mathbf{n}(\tau) = [\cos(\theta(\tau)), \sin(\theta(\tau)), 0]$ specified by an angle θ. Expanding in the angular variables and retaining leading time derivatives gives

$$S_{xy} = \frac{1}{2} \sum_{k,\omega} \chi_{zz}^{-1}(k, \omega) |\phi_z(k, \omega)|^2 - \frac{\gamma_{xy}}{2} \int d\tau_1 \, d\tau_2 \, \partial_\tau \mathbf{n}(\tau_1) \cdot \partial_\tau \mathbf{n}(\tau_2) \ln\left(\frac{\tau_0^2 + (\tau_1 - \tau_2)^2}{\tau_0^2} \right)$$
$$- \frac{uM^2}{8} \int d\tau [i \partial_\tau \mathbf{n} \times \mathbf{n} \cdot \hat{\mathbf{z}} + h_z(\tau)]^2 \quad (6)$$

with $M^2 = \int d^D r \, \phi_0^2(\mathbf{r})$, $h(\tau) = 2 \int d^d r \, \phi_0(r) \, \delta\phi_z(r, \tau)/M^2$, and $\gamma_{xy} = (2\pi)^{-d} \int d^d q \, |\phi_0(q)^2|/\Gamma_q$. We thus obtain the action expected for a rotor with a large moment of inertia (M) in a dissipative environment, precessing in an effective magnetic field caused by the background spin fluctuations. Reference [26] indicates that in the large dissipation limit the subtleties associated with spin quantization may be neglected. A straightforward variational estimate then yields $\langle \mathbf{n}(\tau)\mathbf{n}(\mathbf{0}) \rangle \sim \tau^{-\mathbf{x}}$ with nonuniversal $x > 1/2$, corresponding to a divergent susceptibility.

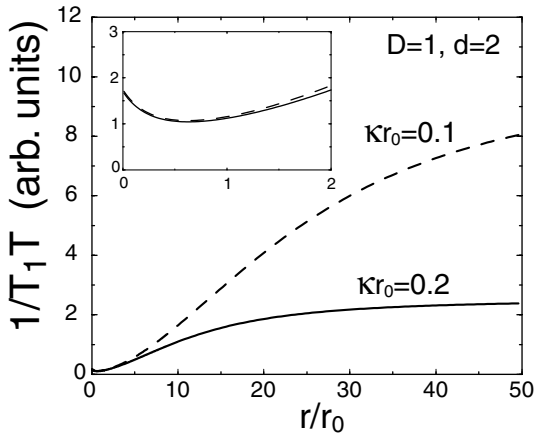

FIG. 2. Dependence of the Gaussian fluctuation contribution to the NMR relaxation rate on the distance from the defect, calculated for $z = 2$, $d = 2$, and $D = 1$ and two distances from criticality. Inset: expanded view of the near-defect ($r \approx r_0$) region.

The presence and fluctuations of the droplet are, in principle, observable via NMR measurements of the spin lattice relaxation rate, $T_1^{-1}(r) \sim T\,\mathrm{Im}\chi(r,\omega)/\omega$, and the local Knight shift. There are two different contributions: from changes, due to the droplet, in the extended "Gaussian" spin fluctuations, and from the presence and tunneling of the droplet itself. The two contributions have very different time scales and position dependences. The Gaussian fluctuations have the characteristic frequency $\omega \sim \kappa^z$ and give rise to the usual divergence of the bulk relaxation rate as criticality is approached. This contribution to $1/T_1T$ is suppressed near the defect (cf. Fig. 2) because the droplet reduces the amplitude of the low energy wave functions in the near-defect region (cf. Fig. 1b). The droplet tunneling processes provide a contribution to $\chi''(r,\omega)$ which is proportional to the square of the droplet amplitude but varies on a much slower time scale, which vanishes exponentially as criticality is approached, so that these processes drop out of the NMR frequency window, appearing instead as a broadening $\propto 1/r_0$ of the NMR spectrum. Details will be given elsewhere [21].

In summary, we have presented a theory of a single defect in a quantum critical system at or above its upper critical dimension. A crucial property is the $1/r$ tail of the droplet extending into the surrounding medium. The ease with which line and plane defects induce regions of local order may be relevant to the small moments observed in heavy fermion systems [1,2]. Our finding that, near criticality in a metallic system, droplets behave in an essentially classical manner leaves no significant parameter regime in which the quantum Griffiths behavior discussed in [12,13] exists. The strong dimensionality dependence of our results has implications for the general issue of Griffiths behavior near quantum criticality. Finally, our results bear on the fundamental question of the Kondo effect near a quantum critical point [15]. A single spin in a nearly critical system will similarly induce a large droplet, which we believe will be prevented from tunneling by dissipative effects.

D. K. M. acknowledges support by the U.S. DOE at the Los Alamos National Laboratory, and A. J. M. thanks D. Khmelnitskii and M. P. A. Fisher for helpful conversations, and acknowledges NSF DMR 00081075, the British EPSRC, Cambridge University, and the ITP at Santa Barbara for support. J. S. acknowledges support by the Ames Laboratory operated for the U.S. DOE by Iowa State University under Contract No. W-7405-Eng-82.

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