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 droplet 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.

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The behavior of 'droplets' of local order in a non-ordered 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 [12,13] and may be related to grain boundaries and other structural defects [3–5]. In a colossal magnetoresistance material, magnetic order was observed to be enhanced near grain boundaries. [6] A related issue is the magnetism induced in high temperature superconductors by apparently non-magnetic substituents such as Zn [7], which have been interpreted [8] as spin droplets induced in a nearly critical system (although other interpretations exist also [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. [12–15]. The problem bears on the fundamental issue of the Kondo effect near a quantum critical point [16]. 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 it 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 $d = 2, 3$ [17,18] and "quantum paraelectric" (i.e. nearly ferroelectric) systems in $d = 3$ [19]. We study defects which couple to the square of the order parameter, i.e. change the 'local $T_c$', and thus create small regions where order is more favored than in the pure system. We address three questions: under which circumstances does the defect create a 'droplet', a region about the defect in which the order parameter is non-vanishing (at least on short time scales)? What is the size and general properties of the droplet? What are the relevant fluctuations? Our work is complementary to that of Vojta and Sachdev [20], who studied a linear coupling of the defect to the order parameter in a quantum critical system below $d_u$. It is also related to the work of Castro-Neto and Jones [3,14], but differs in several important aspects.

Our starting point is a quantum Ginzburg-Landau action for an order parameter field $\phi$. After obtaining its mean field solution we consider fluctuation corrections, which are tractable because the dimension of the system is above $d_u$. Halperin and Varma used a similar approach for a classical system [21]. Our action, in conveniently scaled variables, is, in space and imaginary time:

$$S = S_{\text{dyn}} + \frac{1}{2} \int_0^{E_0/T} d\tau \int d^d x \{ (V(x) + \kappa^2) \phi(x,\tau)^2 + (\nabla \phi(x,\tau))^2 + \frac{1}{2} \phi(x,\tau)^4 \}. \quad (1)$$

Here, $\kappa$ determines the distance of the bulk system to the critical point. We measure lengths in units of the bare correlation length of the problem (typically of the order of a lattice constant) and 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 of the order of a lattice constant) over which $V$ decays in the $D = d - d_d$ transverse directions, and a dimensionless strength $v = -\int d^d r V(r)$ ($v > 0$ corresponds to a local tendency towards order). Here, $r$ refers to the $D = d - d_d$ transverse components of the $d$-dimensional vector $x$, where $d_d = 0, 1, 2$ corresponds to a point, line and plane defect, respectively.

The dynamic term $S_{\text{dyn}}$ takes the general form

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

where the coefficients $c$ and $\Gamma$ depend on whether the system is overdamped (metallic case) or not, on the sym-
metry of the order parameter, and on whether it is conserved. Examples include: (1) the undamped Ising antiferromagnet, with $\Gamma^{-1} = 0$ and $c =$ const; (2) the undamped Ising ferromagnet with a conserved order parameter, $\Gamma^{-1} = 0$ and $c \sim 1/q$; (3) the metallic (overdamped) antiferromagnet $[17,18] \Gamma =$ const; (4) the metallic Ising ferromagnet $\Gamma_q \sim q$. The form of $S_{\text{dyn}}$ combined with the static part of the free energy defines a (mean-field) dynamic exponent $z$ which is $z = 1, 2, 3$ 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 to $d_{\text{eff}} \geq 4$.

We now sketch the essential features of the mean field solution (details will be given elsewhere [22]). We focus only on the transverse dimensions and assume $V(r > a) = 0$ so that for $r > a$ the mean field equation is

$$- \nabla^2 \phi_0 + \kappa^2 \phi_0 + \phi_0^3 = 0.$$  \hspace{1cm} (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 one for $r < a$ and thus depends on the defect strength, $v$. For $\kappa r_0 > 1$ the $\phi^3$ term may be neglected at all $r$ and the solution is the familiar exponentially decaying one. In the more interesting case $\kappa r_0 < 1$ 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. We find (the $g_D$ are constants):

| $D$ | $r < r_0$ | $r_0 < r < \kappa^{-1}$ | $\kappa^{-1} < r$ |
|-----|------------|------------------------|----------------|
| 1   | $g_1 r_0^{-1}$ | $\sqrt{2}/r$ | $\sqrt{2}\kappa e^{-\kappa r}$ |
| 2   | $g_2 \ln \left( \frac{r_0}{r} \right) + g_2' \frac{r_0}{r}$ | $1/r$ | $e^{-\kappa r}/r^{1/2}$ |
| 3   | $g_3 \ln^{1-2} \left( \frac{r}{r_0} \right) / r$ | $e^{-\kappa r}/r^{3/2}$ |
| > 3 | $g_0 r_0^{-1}$ | $r_0^{(D-3)/2} r^{D-2}$ | $e^{-\kappa r}/r^{(D-1)/2}$ |

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 exponential tail of $\phi_0(r)$. Fig. 3a 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. (3) and minimizing with respect to $r_0$. This also determines the binding energy, $E_{\text{bind}}$, of the droplet which forms at temperatures $T < E_{\text{bind}}$. Alternative approaches including scaling, exact solutions ($D = 1$), and numerics give identical results [22]. 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 $D = 2 r_0 \sim e^{1/2v}$ and $E_{\text{bind}} \sim -E_0 e^{-2/v}$. 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 $E_{\text{bind}} \sim -E_0 v^6 (\frac{a}{v^*} - 1)a^{-2}$. The droplet size cannot exceed $\kappa^{-1}$, which yields an estimate for the critical potential $v^*(\kappa) v > v^* = 2\kappa (D = 1)$ and $v > v^* = -2\pi/\log(\kappa a)$ ($D = 2$). The droplet magnetization $M_d$ in the ferromagnetic case is given by the integral of $\phi_0(r)$ which diverges as $\kappa^{1-D}$ (logarithmically in $D = 1$) as criticality is approached. In an antiferromagnetic system with characteristic wave vector $Q$, $M_d \sim |Q|^{1-D}$ which for $D \geq 1$ is a number of order unity even at criticality. We show below that these mean field results are not significantly affected by fluctuations, at least in metallic systems. Gaussian fluctuations may be treated by expanding to quadratic order about the mean field solution, leading to the action:

$$S_{\text{GF}} = S_{\text{dyn}} + \frac{T}{2} \int d^d x \sum_{i\omega_n} \psi(x, i\omega_n) \hat{L} \psi(x, i\omega_n)$$  \hspace{1cm} (4)

where $\hat{L} = \kappa^2 + V(r) + 3\phi_0^2(r) - \nabla_x^2$. $\hat{L}$ 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 attractive center) leads to non-monotonic 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 $r-$dependence is shown for two even parity wave-functions of the Gaussian fluctuations in Fig. [3]. The effect of Gaussian fluctuations on the droplet size and shape may be computed in terms of the difference between the eigenvalues of $L$ and of $k^2 - \nu^2$ and are found [2] not to change the long distance behavior of the droplet (as expected from conventional RG arguments [13]).

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 re-forms. In extended ($d_d > 0$) droplets the important processes are motion 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 [2]. The dynamics of an isolated (not embedded in a critical system) droplet have been previously studied [2]; 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 $\phi(r, \tau) = \phi_0(r)\eta(\tau)$ into Eq. (1) and retain leading time derivatives. We find that the action corresponding to 2N instantons is

$$S_{2N} = \frac{\gamma}{2} \sum_{i \neq j = 1 \ldots N} \log(y_i - y_j)(-1)^{i+j} + 2N \left( \frac{y_0}{\varsigma} + \frac{m}{y_0} \right)$$

$$+ \frac{2N\gamma}{4} \int_{-1}^{1} du \int_{-1}^{1} dv \log(1 + y_0^2(u - v)^2), \quad (5)$$

with $\varsigma = 15E_0/(4E_{bind})$, $m = E_0^2 \sum_q \chi_q^{-2} \phi_0(q)^2$ and $\gamma = E_0 \sum_q \Gamma_q^{-1} \phi_0(q)^2$. The terms proportional to 2N are the action of a single instanton and $y_0$ (determined by minimizing the second and third term of $S_{2N}$) is the duration of an instanton in units of $E_{bind}^{-1}$. Note that both $m$ and $\gamma$ diverge as $k \to 0$ and that $\gamma = 0$ in undamped models. In the weak dissipation ($\gamma \ll 1$) limit the standard macroscopic quantum tunneling analysis [2] leads to $S(y_0) = 8\sqrt{m/\varsigma} + 6m\gamma\varsigma + \mathcal{O}(\gamma^2)$ so 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 $\gamma$ is less than a critical value $\sim 1$ 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 $m/\gamma$. 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 $\gamma$ 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 [22] of the Kondo dynamics of a single spin in a non-critical 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 [3] 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 [14] considered a droplet consisting of a large number of elementary $S = 1/2$ spins locked together by some magnetic interaction in a nearly critical system neglecting the $1/r$ tail of the droplet and studying the effect of dissipation on the bare tunneling rate. Their specific results therefore differ from ours. Their crucial findings were that for antiferromagnetic systems droplets as large as $10^3$ spins could tunnel and that dissipative processes only become important below an exponentially small scale, leaving a wide regime where quantum Griffiths behavior occurs, whereas we find that near criticality dissipation always dominates and quantum effects are suppressed.

In droplets with XY or higher symmetry, rotational fluctuations must be considered. We integrate out the conduction electrons of an action of the type discussed in [22] and assume that $\phi$ is characterized by an amplitude $\phi_0(r)$, obtained by solving Eq. (3), and a direction $n(\tau) = (\cos(\theta(\tau)), \sin(\theta(\tau)), 0)$ specified by an angle $\theta$. Expanding in the angular variables and retaining leading time derivatives gives

$$S_{xy} = \frac{1}{2} \sum_{k, \omega} \chi_z^{-1}(k, \omega) |\phi_z(k, \omega)|^2$$

$$- \frac{\gamma_{xy}}{2} \int d\tau_1 d\tau_2 \partial_\tau \phi_z(\tau_1) \cdot \partial_\tau \phi_z(\tau_2) \ln \left( \frac{\tau_2^2 + (\tau_1 - \tau_2)^2}{\tau_0^2} \right)$$

$$- uM^2 \int d\tau (i\partial_\tau n \times n \hat{z} + h_z(\tau))^2 \quad (6)$$

with $M^2 = \int d^D r \phi_0^2(r) h(\tau) = 2 \int d^D r \phi_0(r) \delta \phi_z(r, \tau)/M^2$ 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. Ref. [23] indicates that in the large dissipation limit the subtleties associated with spin quantization may be neglected. A straightforward variational estimate then yields sub-diffusive long-time behavior, corresponding to a divergent susceptibility.

The presence and fluctuations of the droplet are in principle observable via NMR measurements of the spin lattice relaxation rate, $T_1^{-1}(r) \sim T \text{Im } \chi(r, \omega)/\omega$ and 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 timescales and position dependences. The Gaussian fluctuations have characteristic frequency \( \omega \sim \kappa^2 \) 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 (as shown for example in Fig. 2) essentially 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 timescale, which moreover 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. Further details will be given elsewhere [22].

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 [4]. 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 [3,4] 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 [16]. 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.

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FIG. 2. Dependence of the Gaussian fluctuation contribution to the NMR relaxation rate on 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.

\[ 1/T_1T = \frac{1}{r_0} \]

\[ \kappa = 0.1 \]

\[ \kappa = 0.2 \]

\[ D = 1, d = 2 \]

\[ T_1(T) \]

\[ 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12 \]

\[ 0, 10, 20, 30, 40, 50 \]

\[ \kappa = 0.1 \]

\[ \kappa = 0.2 \]

\[ r/r_0 \]

\[ 0, 10, 20, 30, 40, 50 \]

\[ 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12 \]

\[ 0, 10, 20, 30, 40, 50 \]

\[ \kappa = 0.1 \]

\[ \kappa = 0.2 \]

\[ D = 1, d = 2 \]

\[ 0, 10, 20, 30, 40, 50 \]

\[ 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12 \]

\[ 0, 10, 20, 30, 40, 50 \]

\[ \kappa = 0.1 \]

\[ \kappa = 0.2 \]

\[ D = 1, d = 2 \]

\[ 0, 10, 20, 30, 40, 50 \]
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