Droplets in Disordered Metallic Quantum Critical Systems

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We present a field theory for a structurally disordered magnetic system coupled to a metallic environment near a quantum critical point. We show that close to the magnetic quantum critical point droplets are formed due to the disorder and undergo dissipative quantum dynamics. We show that the problem has a characteristic energy scale, the droplet Kondo temperature, that determines the crossover energy scale from weak to strong coupling. Our results have direct significance for the Griffiths-McCoy singularities of itinerant magnets.

The behavior of itinerant magnets close to quantum critical points (QCP) has been a subject of intense research in the last few years. It has been found experimentally that a broad class of systems show anomalous metallic behavior in the paramagnetic phase \([1]\). Since a large number of such systems are structurally disordered due to chemical substitution the question arises of the importance of disorder for the understanding of the anomalies observed in the experiments. We have proposed recently that the anomalous behavior observed in some of these systems can be understood in terms of Griffiths-McCoy singularities close to a QCP \([2,3]\). These singularities occur in the context of percolation theory on a discrete lattice when clusters of spins tunnel quantum mechanically. In the presence of a metallic environment we have shown that electrons scatter against clusters leading to a \textit{cluster Kondo temperature} associated with their dissipative quantum dynamics \([3]\). We found that while dissipation freezes the clusters when the system is close enough to the QCP, there is still possibility of quantum behavior in a large region in the parameter space around the QCP. In this case small Kondo temperatures can be obtained even for relatively small clusters dropping the requirement of cluster “rarity” as a condition for anomalous magnetic behavior \([3]\). These results put our approach in proximity to the single ion Kondo disorder theories \([4]\).

In a recent paper Millis, Morr and Schmalian (MMS) \([5]\) proposed that a single isolated local perturbation close to a QCP of an itinerant Ising magnet produces large droplets with internal structure that are blocked from tunneling due to dissipative effects. While that theory has similar features to the Griffiths-McCoy scenario proposed by us, their theory is supposed to be valid for clean critical systems with a vanishing small amount of local defects. Experimentally this scenario can be realized by introducing a very small amount of impurities into clean stoichiometric compounds like CeRu\(_2\)Ge\(_2\) \([6]\) or CePd\(_2\)Si\(_2\) \([7]\) and driving the system close to a QCP by application of hydrostatic pressure.

In this work we study the problem of a disordered alloy such as U\(_{1-x}\)Y\(_x\)Pd\(_3\) \([8]\) or UCu\(_{5-x}\)Pd\(_x\) \([9]\) with a finite density of defects or impurities and where the distance from the QCP is controlled by chemical substitution. We show that, for the same field theory studied by MMS, a \textit{finite density} of impurities leads to Griffiths-McCoy singularities in a region close to the QCP. We show that in the presence of disorder the droplet is structureless and its average size is set by the magnetic correlation length, \(\xi\). More importantly, we demonstrate that the droplets have a finite droplet Kondo temperature, \(T_K\), that varies continuously with the distance from the QCP and vanishes when the system is sufficiently close to it. These results are in agreement with our previous \textit{microscopic} analysis of the disordered Kondo lattice model \([3]\) but also apply to other models of strongly correlated electrons such as the Hubbard model \([10]\).

The starting point of our analysis of droplet formation close to a QCP is the Hertz action for a critical itinerant magnetic system in \(d\) spatial dimensions \([11]\) (we use units such that \(\hbar = k_B = 1\)):

\[
S = \frac{1}{2\beta} \sum_{n,q} (\omega_n^2 + \gamma \Gamma_q |\omega_n| + q^2 + r) |\varphi(\omega_n, q)|^2
\]

where \(\omega_n\) and \(q\) are the Matsubara frequency and momentum, respectively, \(\gamma\) is the coupling between the order parameter \(\varphi(x, \tau)\) and the particle-hole continuum, \(\Gamma_q\) gives the momentum dependence of the dissipative coupling \((\Gamma_q = q^{-\zeta})\) with \(\zeta = 0\) for antiferromagnets, \(\zeta = 1\) for clean ferromagnets and \(\zeta = 2\) for disordered ferromagnets). The distance from the QCP is controlled by \(r\). In the ordered phase \(r < 0\) indicating an instability towards long range order and at the QCP we have \(r = 0\). In this work we focus entirely in the paramagnetic phase where \(r > 0\) so that we can parametrize \(r = \xi^{-2}\). Disorder is introduced into the problem as a random variation of \(r\) in real space:

\[
S_{\text{dis}} = -\frac{1}{2} \int dx \int_0^\beta d\tau d\delta r(x) \varphi^2(x, \tau)
\]

which is assumed to be Gaussian distributed with width \(u\), that is, the probability distribution is given by:
\begin{equation}
P(\delta r) \propto \exp \left\{ -\frac{1}{4u} \int dx \ (\delta r(x))^2 \right\} \end{equation}

so that \( \delta r(x) = 0 \) and

\[ \bar{\delta r(x)} \delta r(y) = u \ \delta^d(x - y) \]

where the average is calculated with \([1]\). The reason for the appearance of droplets in the problem is that the Gaussian distribution \([1]\) allows for local values of \( \delta r(x) \) (the tails of the distribution) such that \( r - \delta r(x) < 0 \), that is, it allows for local order even in the absence of long range order. These locally ordered regions in a surrounding paramagnetic media are called droplets.

Since we are not interested in one particular realization of the disorder we study the average free energy using replicas \([11]\). We introduce \( n \) replicas of the order parameter \( \varphi_a \) with \( a = 1, \ldots, n \) and calculate the average free energy, \( F = \langle Z^n - 1 \rangle / n \), taking the limit of \( n \to 0 \) at the end of the calculation. It can be easily shown that a new term is generated in the quantum action:

\[ S_{dis} = -\frac{u}{4} \sum_{a,b} \int dx \int_0^\beta d\tau \int_0^\beta d\tau' \varphi_a^2(x, \tau) \varphi_b^2(x, \tau') . \]

Notice that the disorder not only generates interactions between fields in different replicas but also couples the fields in the imaginary time direction. Our calculations can also be carried out with a non-linear term of the form \( g \varphi^4(x, \tau) \) with no fundamental change in the results. Thus, in order to keep the discussion simple we have dropped this term.

We first study the problem of droplet formation by investigating the static, classical, part of the action. In this case \( \varphi_a(x, \tau) = \psi_a(x) \) where \( \psi_a \) is obtained from the variational solution of the static part of the action:

\[ -\nabla^2 \psi_a(x) + r \psi_a(x) - u_\beta \psi_a(x) \sum_b \psi_b^2(x) = 0. \]  

This equation is quite revealing. If the problem were to be replica symmetric, that is, \( \psi_a(x) = \psi_0(x) \) for all values of \( a \), the last term in \([1]\) would scale like \( n \psi_0^2(x) \) and would vanish in the limit of \( n \to 0 \). This would imply that the only solution in the paramagnetic phase (\( r > 0 \)) is the trivial solution \( \psi_0 = 0 \). Thus, in order for droplets to form in the paramagnetic phase one needs the replica symmetry to be broken. Here we follow Dotsenko \([14]\) who studied the classical problem in detail and assume a non-trivial replica solution such that for \( a = 1, \ldots, k \) we have \( \psi_a(x) = \psi_k(x) \) while \( \psi_a(x) = 0 \) for \( a = k + 1, \ldots, n \). Here \( k > 1 \) is an integer that determines the degree of the symmetry breaking process. Using this particular solution we see that \([1]\) can be rewritten as:

\[ -\nabla^2 \psi_k(x) + r \psi_k(x) - u_\beta k \psi_k^3(x) = 0. \]  

This equation is non-linear Schrödinger equation and can be thought as the equation for a classical particle moving in the potential shown in Fig.1.

![FIG. 1. Replica potential.](image)

A naive conclusion from this discussion would be that the “energy” would be minimized for \( \psi = \pm \infty \), a solution that is clearly unphysical. It should be kept in mind that the replicated action is not the actual free energy of the problem; the latter is only obtained after we take the limit of \( n \to 0 \) at the end of the calculation (this fact is a standard consequence of the application of the replica method \([11]\)). Dotsenko has shown that the stable static solutions of this problem are the maxima of Fig.1. Mathematically this can be proved by showing that all the eigenvalues of the fluctuation matrix (the Hessian) are real and positive \([12]\). The maxima are associated with the two possible configurations of the droplet (spin configurations pointing up and down). Equation \([1]\) can be rescaled if we define

\[ \psi_k(x) = \sqrt{\frac{r}{u_\beta k}} \phi(\sqrt{r}x) \]  

so that \( \phi(z) \) obeys a scale independent equation:

\[ -\nabla^2 \phi(z) + r \phi(z) - \phi^3(z) = 0 \]  

where \( z = \sqrt{r}x \). The proper boundary conditions are \( \phi(0) = \text{constant} \) and \( \phi(z \to \pm \infty) = 0 \). Equation \([5]\) has exponentially decaying solutions for \( x \gg 1/\sqrt{r} \) and is smooth for \( x < 1/\sqrt{r} \). This can be contrasted with the solution found by MMS for a local defect in which the droplet is such that for \( x < 1/\sqrt{r} \) the droplet profile decays like \( 1/x \). It is the \( 1/x \) decay that makes the MMS problem special \([3]\). Here such a behavior does not occur in \( d < 4 \). Moreover, it is clear that the size of the droplet is the magnetic correlation length:

\[ R \approx \frac{1}{\sqrt{r}} = \xi . \]

Thus droplets become arbitrarily large close to the QCP.

The action for the static droplet can be calculated by substitution of \([4]\) into the original action, and the free energy, after summing over the replicas, reads \([12]\):

\[ \text{This equation is non-linear Schrödinger equation and can be thought as the equation for a classical particle moving in the potential shown in Fig.1.} \]
\[
\frac{F_D}{V} \approx -ur'^{d/2}\exp\left\{-\frac{\sqrt{2-d/2}E_2}{4u}\right\}
\]

where \(E_N = \int d^d z \phi^{2N}(\hat z)\) and \(V\) is the volume of the system. As pointed out by Dotsenko the non-analytic, non-perturbative, dependence of the free energy on the disorder strength \(u\) for \(d < 4\) shows that the static field theory reproduces the classical Griffiths result in a percolating lattice [13]. Obviously in order to study quantum or Griffiths-McCoy singularities [14] we have to allow the droplet to tunnel between the two maxima of the potential in Fig.4.

In order to study the tunneling of the droplet we assume a rigid droplet approximation [3]:

\[
\varphi(x, \tau) = \psi_k(x)X(\tau)
\]

where all the dynamics is encapsulated in \(X(\tau)\). This choice assumes that the droplet tunnels as a whole. Direct substitution of (3) into the action leads to:

\[
Z[X] \approx \int DX(\tau) e^{-r^2-d/2E_2\mathcal{F}[X]/u}
\]

where

\[
\mathcal{F}[X] = \frac{1}{\beta} \int_0^\beta d\tau \left\{ \frac{M}{2} \left(\frac{dX(\tau)}{d\tau} \right)^2 + \frac{X^2(\tau)}{2} \right\}
- \frac{1}{4\beta} X^2(\tau) \int_0^\beta d\tau' X^2(\tau')
+ \frac{\eta}{4\pi} \int_{-\infty}^{+\infty} d\tau' \frac{(X(\tau) - X(\tau'))^2}{(\tau - \tau')^2}
\]

is the replica free energy for \(X(\tau)\). The coefficients in (3) are:

\[
M = \frac{E_1}{E_2} r^{-1}
\]
\[
\eta = \frac{\gamma G_\zeta}{E_2} r^{-(1+\zeta/2)}
\]

that can be associated with the “particle” mass and dissipation coefficient, respectively. Here \(G_\zeta = \int d^d q q^{-\zeta} |\phi_q|^2\), \(\phi_q\) is the Fourier transform of \(\phi(z)\) and periodic boundary conditions are assumed: \(X(\tau + \beta) = X(\tau)\). Observe that \(\mathcal{F}\) describes a Caldeira-Leggett action [4] for the motion of a dissipative particle in a non-local, non-linear, potential which, for slowly varying configurations of \(X(\tau)\) reduces to the potential of Fig.4.

Assuming that most of the time the field is in the equilibrium configuration \(X(\tau) = \pm 1\) the problem becomes equivalent to the problem of a two-level system coupled to a dissipative environment [16].

The amount of damping in the tunneling of the droplet can be estimated by comparing the parameters in (3). We have weak damping when \(\eta \ll \omega_0 M\) while for strong damping one has \(\eta \gg \omega_0 M\) (\(\omega_0 = 2\) is the undamped frequency of motion in our dimensionless units). Notice that the crossover from weak to strong dissipation occurs at \(r = r_c\) where (using (3))

\[
r_c \approx \left( \frac{\gamma G_\zeta}{2E_1} \right)^{2/\zeta}
\]

which indicates that close to the QCP \((r < r_c)\) the droplet motion is highly damped. The tunneling splitting between the two configurations \(X = \pm 1\) is given by [16]:

\[
\Delta = \omega_{cl} e^{-\frac{8M\omega_{cl}}{\zeta}}
\]

where \(\omega_{cl}\) is the classical frequency of oscillation. On the one hand in the weakly dissipative regime \((r > r_c)\) one has \(\omega_{cl} \approx \omega_0\) and therefore the tunneling splitting is:

\[
\Delta_{r>r_c}(r) \approx 2e^{-a/r}
\]

where \(a = 16E_1/E_2\) is a universal constant. On the other hand in the strongly dissipative regime \((r < r_c)\) we have \(\omega_{cl} \approx M\omega_0^2/\eta\) and therefore

\[
\Delta_{r<r_c}(r) \approx \frac{4\sqrt{2}}{\gamma} e^{-br^\zeta}
\]

where \(b = 32E_1/\gamma G_\zeta\) is a non-universal constant. For antiferromagnets \((\zeta = 0)\) the tunneling splitting is constant close to the QCP while it vanishes in the case of ferromagnets \((\zeta = 1, 2)\). Another important parameter is the Caldeira-Leggett dissipative coupling that is given by:

\[
\alpha(r) = \frac{2\eta}{\pi} = \left(\frac{r_0}{r}\right)^{1+\zeta/2}
\]

where we used (3) and defined

\[
r_0 = \left( \frac{2\gamma G_\zeta}{\pi E_2} \right)^{1/(1+\zeta/2)}.
\]

Observe that the dissipative coupling diverges at the QCP. As is well-known this problem has a characteristic crossover energy scale that can be associated with the Kondo temperature, \(T_K\), of an anisotropic Kondo impurity model [16]. This energy scale separates the region of strong and weak coupling and for \(\alpha < 1\) is given by:

\[
T_K(r) \approx W \left( \frac{\Delta(r)}{W} \right)^{-1/(1+\zeta/2)}
\]

where \(W\) is a cut-off energy scale. For \(\alpha > 1\) we have \(T_K = 0\) and the droplet is frozen. Notice that according to (3) the freezing of the droplet occurs for \(r < r_0\). This indicates that close to the QCP droplets are frozen. Observe that \(r_0\) given in (12) is a non-universal quantity which depends on parameters that cannot be obtained in
a continuum field theory. Depending on the microscopic parameters the freezing of the droplets can occur in the region of weak damping if \( r_0 > r_c \) or strong damping if \( r_0 < r_c \), affecting the value of the tunneling splitting given in (9) and (10). Thus \( T_K(r) \) is finite and a continuous function of the distance from the QCP in agreement with our previous analysis [3]. This should be contrasted with the result obtained by MMS [5] where \( T_K = 0 \) in all the parameter space. In fact for \( r \gg r_0 \) the droplets become free to tunnel [2]. The phase diagram is shown in Fig. 2.

![Phase Diagram](fig2.png)

**FIG. 2.** Phase diagram as a function of the parameter \( r \): the system is ordered for \( r < 0 \); droplets are frozen in the paramagnetic phase for \( 0 < r < r_0 \) and can quantum tunnel for \( r > r_0 \).

Direct comparison of [13] with our previous results in Ref. [3] indicates that the two problems map into each other if \( N \propto \xi^2 \) where \( N \) is the number of spins in the cluster. Another interesting consequence of our calculation is the sharp contrast between the case of ferromagnetic and antiferromagnetic droplets. For antiferromagnetic droplets (\( \zeta = 0 \)) the dissipation coefficient in (11) scales with \( \xi^2 \) while in the case of a clean ferromagnet (\( \zeta = 1 \)) we find \( \alpha \propto \xi^4 \) indicating stronger damping. For a ferromagnetic system with diffusive electrons (\( \zeta = 2 \)) damping becomes even stronger with \( \alpha \propto \xi^4 \). This indicates, in agreement with our previous analysis [3], that dissipation is more important in the case of ferromagnetic droplets than in the case of antiferromagnetic ones. Since the great majority of systems studied experimentally are of the antiferromagnetic type [1], our results indicate that dissipation does not freeze the droplets in a region of the parameter space around the QCP.

A question that comes to mind is the reason for the difference between our results and the ones obtained by MMS [5]. We claim that our approaches are valid in different regimes. A clear way to understand this difference is to perform the same calculation for a Poisson distribution of Dirac delta potentials [7]. In this case the problem is characterized by two physical parameters: the density of impurities \( \rho \) and the strength of the potential \( V \). A universal Gaussian distribution like the one discussed in this paper is obtained by taking the limit of \( \rho \to \infty \) and \( V \to 0 \) so that \( u = \rho V^2 \) is constant. On the other hand the single impurity limit studied by MMS is obtained by letting \( \rho \to 0 \).

In summary, we have studied the problem of droplet formation and dynamics close to a QCP of a disordered itinerant Ising magnet. We find that the droplets have a finite Kondo temperature (associated with their dissipative quantum dynamics) that varies continuously with the distance from the QCP. We show that the characteristic Kondo temperature of the droplet is finite except in a non-universal region (dependent on microscopic details) close to the QCP. These results are in agreement with our previous analysis of quantum Griffiths-McCoy singularities in the disordered Kondo lattice model and extends the validity of our results to other strongly correlated systems.

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