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Convergence of energy scales on the approach to a local quantum critical point

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We find the emergence of strong correlations and universality on the approach to the quantum critical points of a two impurity Anderson model. The two impurities are coupled by an inter-impurity exchange interaction $J$ and direct interaction $U_{12}$ and are hybridized with separate conduction channels. The low energy behavior is described in terms of renormalized parameters, which can be deduced from numerical renormalization group (NRG) calculations. We show that on the approach to the transitions to a local singlet and a local charged ordered state, the quasiparticle weight factor $z \to 0$, and the renormalized parameters can be expressed in terms of a single energy scale $T^*$. The values of the renormalized interaction parameters in terms of $T^*$ can be predicted from the condition of continuity of the spin and charge susceptibilities, and correspond to strong correlation as they are greater than or equal to the effective band width. These predictions are confirmed by the NRG calculations, including the case when the onsite interaction $U = 0$.

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There is increasing interest, both experimentally and theoretically, in strongly correlated electron systems which have anomalous behavior in the region of a $T = 0$ or quantum phase transition (for a recent review see [1]). The generalizations of the Wilson renormalization group approach to zero temperature transitions, initiated by the early work of Hertz and followed up by others [2], have not provided a comprehensive framework to explain many examples of quantum critical behavior. Particularly challenging is the range of anomalies observed at quantum critical points (QCP) in heavy fermion materials, which have been induced by lowering the transition temperature of a magnetically ordered state to zero by pressure, alloying or in some cases by an applied magnetic field [1,3,4].

One possible mechanism that has been put forward for some heavy fermion systems is that, at the critical point, there is a breakdown of the Kondo screening such that the associated Kondo resonance disappears [1,4]. This would imply that the f-like quasiparticles no longer contribute the Fermi surface, so that the Fermi surface would shrink from a large to a small one, containing only the itinerant non-f electrons. It is difficult to test this conjecture for a lattice model of this situation using the theoretical techniques currently available. There is, however, a two impurity Kondo model which has been shown to have a quantum critical point [3,4], which might throw some further light on this particular mechanism. In this Letter, we study a related two impurity model using a combination of renormalized perturbation theory (RPT) and numerical renormalization group (NRG) calculations. Using these techniques we predict that a single energy scale $T^*$ emerges as the critical point is approached, such that at the critical point $T^* = 0$, and the quasiparticle Kondo resonance disappears. These results lead to a new perspective on the two impurity model, and evidence supporting the conjectures that a quantum critical point can be associated with the collapse of the Kondo quasiparticle resonance.

The Hamiltonian of the model we will study has the form, $\mathcal{H} = \sum_{\alpha=1,2} \mathcal{H}_\alpha + \mathcal{H}_{12}$ where $\mathcal{H}_\alpha$ corresponds to an Anderson impurity model in channel $\alpha$ given by

$$\mathcal{H}_\alpha = \sum_{\sigma} \epsilon_{d,\sigma} d_{\alpha,\sigma}^\dagger d_{\alpha,\sigma} + \sum_{k,\sigma} \epsilon_{k,\alpha} c_{k,\alpha,\sigma}^\dagger c_{k,\alpha,\sigma} + U_{\alpha} n_{d,\alpha,\uparrow} n_{d,\alpha,\downarrow}$$

where $d_{\alpha,\sigma}^\dagger$, $d_{\alpha,\sigma}$, are creation and annihilation operators for an electron at the impurity site in channel $\alpha$, where $\alpha = 1, 2$, and spin component $\sigma = \uparrow, \downarrow$. The creation and annihilation operators $c_{k,\alpha,\sigma}^\dagger$, $c_{k,\alpha,\sigma}$ are for partial wave conduction electrons with energy $\epsilon_{k,\alpha}$ in channel $\alpha$.

The second part of the Hamiltonian $\mathcal{H}_{12}$ describes the interaction between the impurities in the two channels, which we take in the form of a direct Coulomb term $U_{12}$ and an Heisenberg exchange term,

$$\mathcal{H}_{12} = U_{12} \sum_{\sigma} n_{d,1,\sigma} \sum_{\sigma'} n_{d,2,\sigma'} + 2JS_{d,1} \cdot S_{d,2},$$

where $J > 0$ for an antiferromagnetic coupling.

For the model with $U_{12} = 0$ there is a competition between two modes of screening of the impurity spins; by Kondo screening in the channel directly hybridized to each impurity or by the direct antiferromagnetic coupling between the impurities. The Kondo screening by
the individual channels predominates for small $J$, and the local screening for large $J$. NRG studies \cite{1} of the Kondo version of the symmetric model have shown that there is a critical point between these competing terms at a value $J = J_c$, where $J_c$ is proportional to the Kondo temperature $T_K$ of an isolated impurity ($J = 0$). It was also shown there is a divergence of the impurity specific heat coefficient at the transition point and an anomalous $\log(2)/2$ entropy. Conformal field theory \cite{3,10} and bosonization studies \cite{3} have clarified the conditions for such a transition to occur and shown that the staggered susceptibility diverges at the transition point.

The model with $J = 0$, $U_{12} \neq 0$, has been used to describe two capacitively coupled quantum dots, and NRG studies have revealed a second type of transition at a critical value of $U_{12} = U_{12}^c$ such that for $U_{12} > U_{12}^c$ there is a breaking of local charge order \cite{11}. Further recent NRG studies of both types of transitions have been reported using related versions of this model to describe the electron transport in double quantum dots \cite{12,10}.

In the renormalized perturbation theory \cite{17}, the impurity retarded Green’s function $G_{d,\alpha,\sigma}(\omega)$ is re-expressed as $G_{d,\alpha,\sigma}(\omega) = z_{\sigma}G_{d,\alpha,\sigma}(\omega)$, where $G_{d,\alpha,\sigma}(\omega)$ is the quasiparticle Green’s function given by

$$G_{d,\alpha,\sigma}(\omega) = \frac{1}{\omega - \epsilon_d + i\Delta - \Sigma_\sigma(\omega)}$$

and the renormalized parameters, $\tilde{\epsilon}_d$ and $\tilde{\Delta}$ are given by

$$\tilde{\epsilon}_d = z(\epsilon_d + \Sigma_\sigma(0)), \quad \tilde{\Delta} = z\Delta,$$

where $z = 1/(1 - \partial\Sigma_\sigma(\omega,0)/\partial \omega)$ evaluated at $\omega = 0$ and $\Delta = \pi \sum_k |V_k|^2 \delta(\epsilon_k)$. We have taken the two channels to be equivalent and have dropped the channel index.

In working with the fully renormalized quasiparticles, it is appropriate to use the renormalized or effective interactions between the quasiparticles which we identify with the renormalized local four vertices $\Gamma_{\alpha,\beta,\alpha',\beta'}(\omega_1, \omega_2, \omega_3, \omega_4)$ in the zero frequency limit, eg. $\tilde{U}_a = z^22\Gamma_{\alpha,\beta,\alpha',\beta'}(0,0,0,0)$ \cite{17}.

The effective Hamiltonian which describes the low energy excitations corresponds to the original model given in equations (1) and (2) with the parameters replaced by the renormalized values, and the interaction terms have to be normal ordered. For the complete renormalized perturbation expansion to include higher energy scales, counter terms have also to be included to cancel off any further renormalizations \cite{17}.

The quasiparticle interaction terms do not contribute to the linear specific heat coefficient $\gamma$ of the impurities, which is given by

$$\gamma = 4\pi^2 \tilde{\rho}^{(0)}(0)/3, \quad \tilde{\rho}^{(0)}(\omega) = \Delta/\pi \frac{\omega - \epsilon_d}{(\omega - \epsilon_d)^2 + \Delta^2}.$$  

Exact results for the spin susceptibility and charge susceptibilities \cite{18}, $\chi_s$ and $\chi_c$, are given by

$$\chi_s = 4\pi^2 \tilde{n}_s \tilde{\rho}^{(0)}(0), \quad \chi_c = 4\pi^2 \tilde{n}_c \tilde{\rho}^{(0)}(0),$$

and the phase shift $\delta = \tan^{-1}(\Delta/\epsilon_d)$ per spin per channel.

We consider first of all the symmetric model with $U_{12} = 0$. When $J = 0$ the model corresponds to two independent Anderson models and the low energy behavior corresponds to a local Fermi liquid in terms of the two renormalized parameters $\tilde{\Delta}$ and $\tilde{U}$.

When we switch on and increase an antiferromagnetic coupling $J$ this quasiparticle Fermi liquid picture breaks down at a particular coupling $J = J_c$, when the quasiparticle weight $z \to 0$ implying $\tilde{\Delta} \to 0$. This in turn implies that the specific heat coefficient $\gamma$ given by Eq. (5) diverges at this point. However, as we approach this point we would not expect the local uniform spin and charge susceptibilities to diverge as these susceptibilities are suppressed by an antiferromagnetic coupling and the critical fluctuations occur in the staggered spin channel. From Eq. (7) this can only be avoided if in turn the coefficients $\tilde{n}_s \to 0$ and $\tilde{n}_c \to 0$ at the same point, so the product with the singular part remains finite. Assuming $\tilde{U}_{12} = 0$ these conditions imply

$$\tilde{J} \to 2\pi\tilde{\Delta}, \quad \tilde{U} \to \pi\tilde{\Delta}, \quad \text{as} \quad J \to J_c.$$  

We can define an energy scale $T^*_s$ via $\pi\tilde{\Delta}(U,J) = 4T^*_s$, such that $T^*_s$ evolves continuously from the value $T_K$ for $J = 0$. This implies that on approach to the critical point the renormalized parameters can all be expressed in terms of this single energy scale, $\tilde{J}/2 = \tilde{U} = \pi\tilde{\Delta} = 4T^*_s$.

We can apply precisely the same arguments to the model with finite $U_{12}$ and $J = 0$, which has a local charge ordered transition as $U_{12}(>0)$ is increased to a critical value $U_{12}^c$. Assuming $J = 0$, we find

$$\tilde{U}_{12} \to \pi\tilde{\Delta}, \quad \tilde{U} \to -\pi\tilde{\Delta}, \quad \text{as} \quad U_{12} \to U_{12}^c.$$  

Using the RPT approach \cite{18} we can calculate the exact asymptotic behavior of the impurity retarded self-energy $\Sigma(\omega,T)$ for $\omega,T << T_K^*$ from the second order calculation of $\Sigma(\omega,T)$ as $\text{Im} \Sigma(\omega,T) = \text{Im} \Sigma(\omega,T)/z$. The result is

$$\Sigma(\omega,T) = \frac{-i\pi^2 I\Delta}{64} \left[ \left( \frac{\omega}{T^*_s} \right)^2 + \left( \frac{\pi T}{T^*_s} \right)^2 \right],$$

where $I = (2\tilde{U}^2 + 3\tilde{J}^2 + 4\tilde{U}_{12}^2)/(\pi\Delta)^2$, so $I \to 14$ as $J \to J_c$ and $I \to 6$ as $U \to U_{12}^c$.

We have shown in earlier work how the renormalized parameters can be deduced from an analysis of the low energy fixed point of an NRG calculation \cite{18,19}, and we apply the same procedure for this model to calculate
the low energy behavior and test the predictions given in Eqs. 8 and 9. In Fig. 1 we give results for the ratio of $J/J_c$ for $U/\pi \Delta = 0, 0.5, 1, 2, 6$. It can be seen that as $J \to J_c$, $\bar{U}/\pi \Delta \to 1$ in cases including the case $U = 0$, so that strong correlation result emerges even in the weak coupling case on the approach to the critical point. In the right panel of Fig. 2 the corresponding values of $\tilde{J}/\pi \Delta$ are shown and all converge to the limiting value $\tilde{J}/\pi \Delta = 2$, which confirms the predictions given in Eqn. 9. The results also apply for the model with $U_{12} \neq 0$ as it is found that $\bar{U}_{12}/\pi \Delta \to 0$ as $J \to J_c$.

At $J = J_c$ there is a discontinuous change in the NRG fixed point as the two impurities decouple from the conduction band on the lowest energy scale. The phase shift $\delta$ changes from $\pi/2$ to 0 due to the singularity developing in the self-energy of the impurity Green’s functions. For $J > J_c$, $z = 0$ and the previous analysis based on

the assumption of analyticity of the self-energy at $\omega = 0$ breaks down. However, in this regime the low energy behavior still corresponds to a Fermi liquid. We can retain Eqs. (7) and (5) as a description of a local Fermi liquid and treat the first conduction site in the NRG chain as an effective impurity. We can then derive effective renormalized parameters as for $J < J_c$, but we have to take into account that the hybridization is now to a modified conduction chain. The renormalized quantity $\hat{\Delta}$ is no longer equal to $z\Delta$, so in using it to define an energy scale $T^*$ we distinguish it from the values for $J < J_c$, by $4T^*_s = \pi \Delta$.

In Fig. 3 we show the results for the renormalized parameters over the range through the transition point as a function of $J/J_c$ for $U/\pi \Delta = 5$. It can be seen that $\bar{J}/\bar{U}$ is continuous through the transition and takes the predicted value 2 at $J = J_c$. The curves for $T^*_s$ and $T^*_c$ approach the critical point in a similar way proportional to $(J-J_c)^2$ so that it seems reasonable to identify them as a single energy scale $T^*$. The results shown were found to be universal in the strong correlation regime $U/\pi \Delta > 3$.

The value of $\tilde{\eta}_s$, which is the Wilson ratio, is shown as a function of $J/J_c$ in Fig. 4(left). The corresponding spin susceptibility $\chi_s(U,J)/\chi_s(U,0)$, as a function of $J/J_c$ for $U/\pi \Delta = 5$. The value of $\tilde{\eta}_s$ depends on the difference between the renormalized parameters which are very small in this regime, so any
errors in the determination of the parameters become significant. As \( J \) is increased to \( J/J_c = 0.95 \) there is an almost linear decrease with \( J/J_c \). For \( J/J_c > 1.05 \) the susceptibility appears to fall off more slowly with increase of \( J/J_c \). An interpolation between the two regimes, as shown in Fig. 4 (right), suggests that there could be a peak at the critical point \( J = J_c \), but it is very sensitive to the range of the interpolation regime.

\[ \tilde{\Delta} \]

FIG. 5. (Color online) A plot of \( \tilde{\Delta}/\Delta \) (left) and \( \tilde{U}/\pi\tilde{\Delta} \) (circles) and \( \tilde{U}_{12}/\pi\tilde{\Delta} \) (stars) (right) as a function of \( U_{12}/U \) in the approach to the charge order transition for \( U/\pi\tilde{\Delta} = 5 \).

Results for the transition to the local charge ordered state for the model with \( U_{12} \neq 0 \) and \( J = 0 \) are shown in Fig. 5 for \( U/\pi\tilde{\Delta} = 5 \) as a function of \( U_{12}/U \). As \( U_{12} \) is increased there is a point \( U_{12} = U \) with SU(4) symmetry where \( \tilde{U}_{12} = \tilde{U} = \pi\Delta/3 \), which is predicted from the fact that for large \( U \) both the spin and channel fluctuations are suppressed. The critical point occurs for \( U > U_{12} \), where \( \tilde{\Delta} \rightarrow 0 \) implying \( z \rightarrow 0 \) and the disappearance of the resonance at the Fermi level. There is a rapid reduction in \( \tilde{U}/\pi\tilde{\Delta} \) from the SU(4) point to a value -1 at the transition and a commensurate increase in the value of \( \tilde{U}_{12}/\pi\tilde{\Delta} \) to the value 1, in complete agreement with the predictions based on Eqn. (7). As the quantum critical point (QCP) is approached we again have a single energy scale \( T^* \) such that \( \tilde{U}_{12} = \tilde{U} = 4T^*/\pi, \tilde{J} = 0 \), which are also found to apply for the model with finite \( J \) as \( J/\pi\tilde{\Delta} \rightarrow 0 \) at the transition.

In summary, we see that universality appears on the approach to the quantum critical points, such that the renormalized parameters specifying the low energy behavior can be expressed in terms of a single energy scale \( T^* \). At the critical points \( T^* \rightarrow 0 \) the quasiparticle weight factor \( z \rightarrow 0 \) and the spectral density of the impurity levels at the Fermi level goes to zero. The quasiparticle interactions are equal or greater than the renormalized effective band width \( \pi\Delta \), as in the strong correlation regime. The arguments used here should be generally applicable to models of heavy fermions as all the susceptibilitys in Fermi liquid theory at \( T = 0 \) take the form \( \chi_\alpha \propto \tilde{\rho}(0)\tilde{\eta}_\alpha \) where \( \tilde{\rho}(0) \) is the density of states of the non-interacting quasiparticles at the Fermi level and \( \tilde{\eta}_\alpha \) is a factor which depends on the interactions between the quasiparticles. If the specific heat coefficient, which is proportional to \( \tilde{\rho}(0) \) diverges at the QCP and the susceptibility \( \chi_\alpha \) is finite, then \( \tilde{\eta}_\alpha = 0 \) gives a constraint on the quasiparticle interactions. The emergence of a single low energy scale \( T^\ast \) means that the low energy dynamic response functions would have the form \( F(\omega/T^*, T/T^*) \). This would be a natural precursor of \( \omega, T \) scaling because as \( T^* \rightarrow 0 \), it would be expected to go over to a form \( T^* f(\omega/T, 1) \). Calculation of the renormalized parameters from the NRG within a dynamical mean field theory for a lattice model would require the self-consistent solution of the effective band conduction density of states for a two band model.

Some recent interesting experiments have set out to examine the QCP in a two impurity Kondo model by measuring the current between a cobalt atom on an STM tip and a cobalt atom on a metal surface [20]. The results are given as a function of the bias voltage so are under non-equilibrium conditions. There is a direct hybridization term between the cobalt atoms which is not in our model but could be included. Once the renormalized parameters have been determined it is possible to calculate precisely the differential conductance at low bias voltage, using the Keldysh version of the renormalized perturbation theory. This approach could be used to calculate the onset of the splitting of the Kondo resonance seen in these experiments in a similar way to the calculation of the onset of the splitting in a magnetic field in a quantum dot [21].

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