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Friedel oscillations and the Kondo screening cloud

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We show that the long-distance charge-density oscillations in a metal induced by a weakly coupled spin-1/2 magnetic impurity exhibiting the Kondo effect are given, at zero temperature, by a universal function $F(r/\xi_K)$, where r is the distance from the impurity and ξ_K is the Kondo screening cloud size $\equiv \hbar v_F/(k_B T_K)$, where v_F is the Fermi velocity and T_K is the Kondo temperature. F is given by a Fourier-like transform of the T matrix. Analytic expressions for $F(r/\xi_K)$ are derived in both limits $r \ll \xi_K$ and $r \gg \xi_K$ and F is calculated for all r/ξ_K using numerical methods.

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The interaction of a single magnetic impurity with the conduction electrons in a metal is often described by the Kondo model,

$$H=\sum_{\vec{k}\alpha}\varepsilon(\vec{k})\psi^\dagger_{\vec{k}\alpha}\psi_{\vec{k}\alpha}+J\sum_{\vec{k},\vec{k}'\alpha\beta}\psi^\dagger_{\vec{k}\alpha}\frac{\vec{\sigma}_{\alpha\beta}}{2}\psi_{\vec{k}'\beta}\cdot\vec{S}. \qquad (1)$$

In general, we also include a potential scattering term in the Hamiltonian: $H\rightarrow H+V\Sigma_{\vec{k},\vec{k}'\alpha}\psi^\dagger_{\vec{k}\alpha}\psi_{\vec{k}'\alpha}$. This model exhibits a remarkable crossover from weak- to strong-coupling behavior as the energy scale is lowered through the Kondo temperature, $k_BT_K\approx\mathcal{D}\exp(-1/\lambda_0)$, where $\mathcal{D}$ is an ultraviolet cutoff scale (such as a bandwidth) and λ_0 is the dimensionless bare coupling constant ($=J\nu$, where ν is the density of states per spin). For a review, see, for example, Chap. 4 of Ref. 1. The renormalized Kondo coupling, $\lambda(E)$, becomes of O(1) at $E\sim k_BT_K$. While physics at energy scales $E\gg k_BT_K$ is given by weak-coupling perturbation theory, at $E\ll k_BT_K$ the physics is governed by the strong-coupling fixed point corresponding to a screened impurity and a $\pi/2$ phase shift for the low-energy quasiparticles.

The *length* dependence of Kondo physics is much less well understood. It is generally expected that physical quantities exhibit a crossover at a length scale $\xi_K\equiv\hbar v_F/(k_BT_K)$ (where v_F is the Fermi velocity), which is typically in the range of 0.1–1 μm. (We henceforth set $\hbar$ and k_B to 1.) For a review, see Sec. 9.6 of Ref. 1. See Refs. 2–4 for original work on the subject. However, such a crossover at this long length scale has never been observed experimentally and has sometimes been questioned theoretically. One way of observing this length scale is through the density oscillations around a magnetic impurity.[2,3,5,6] It was pointed out in Ref. 2 that these should only approach the standard Friedel form at distances $r\gg\xi_K$, with a form at shorter distances controlled by the $\mathcal{T}$ matrix. However, experimental data so far do not seem to support this expectation,[3] yielding much shorter characteristic lengths. (See also Refs. 6 and 7.) One purpose here is to present a more complete theoretical treatment of these density oscillations, since scanning tunneling microscopy (STM) of magnetic ions on metallic surfaces provides a new experimental technique by which they might now be measured. Alternative approaches to observing this fundamental length scale involve experiments on mesoscopic structures with dimensions of $O(\xi_K)$.[8]

We focus on the case of an $S=1/2$ impurity and a spherically symmetric dispersion relation [normally $\varepsilon(\vec{k})=k^2/2m-\varepsilon_F$]. We consider this model in dimension $D=1$, 2, or 3.

There are two reasons why one might be skeptical that the length scale ξ_K would show up in the charge density. One is the idea of "spin-charge" separation in $D=1$. The Hamiltonian of Eq. (1) in any dimension can be mapped into a one-dimensional (1D) model by expanding in spherical harmonics and using the fact that only the s-wave harmonic interacts with the impurity in the case of a δ-function interaction. The low-energy degrees of freedom of noninteracting 1D electrons can be separated into decoupled spin and charge excitations using bosonization. It is possible to write the Kondo interaction in terms of the spin degrees of freedom only, hence one might expect the charge density to be unaffected by the Kondo interaction. The fallacy in this argument is that the charge density at location r in the 1D model contains a term $\psi^\dagger_{L\alpha}(r)\psi_{R\alpha}(r)\exp(-2ik_Fr)+\text{H.c.}$, where R and L label right and left movers. Standard bosonization methods imply that this term involves both spin and charge bosons: $\sin(\sqrt{2\pi}\phi_c+2k_Fr)\cos[\sqrt{2\pi}\phi_s(r)]$. This is unlike the term $\psi^\dagger_{L\alpha}(r)\psi_{L\alpha}(r)$, which only involves the charge boson.

Another reason why one might expect no interesting Friedel oscillations follows from consideration of the particle-hole (p-h) symmetric case. This symmetry is exact, for example, in a nearest-neighbor tight-binding model at 1/2 filling with the Kondo coupling occurring at the origin only and no potential scattering. Then it can easily be proven that $\langle\psi^\dagger_{j\alpha}\psi_{j\alpha}\rangle=1$ for all sites j. However, a realistic model always breaks particle-hole symmetry. This can be achieved by taking a non-p-h symmetric dispersion relation, for instance moving the density away from 1/2 filling in the tight-binding model. Alternatively, potential scattering can be included in the model. Then, p-h symmetry is broken even if the dispersion relation does not break it.

We find for the density oscillations at zero temperature and $r\gg1/k_F$,

$$\rho(r)-\rho_0 \to \frac{C_D}{r^D}[\cos(2k_F r-\pi D/2+2\delta_P)F(r/\xi_K) - \cos(2k_F r-\pi D/2)]. \quad (2)$$

Here $F(r/\xi_K)$ is a universal scaling function *that is the same for all D*, δ_P is the phase shift at the Fermi surface produced by the potential scattering, $C_3=1/(4\pi^2)$, $C_2=1/(2\pi^2)$, and $C_1=1/(2\pi)$. In general, there are nonzero oscillations but they vanish exactly in the *p-h* symmetry case for $D=1$, where $\delta_P=0$, $k_F=\pi/2$, and r is restricted to integer values, corresponding to a tight-binding model at 1/2 filling. In the limit of zero Kondo coupling, $F=1$ and we recover the standard formula for Friedel oscillations produced by a potential scatterer (in the s-wave channel only). For a small bare Kondo coupling, $\lambda_0 \ll 1$, $F(r/\xi_K)$ is close to 1 at $r\ll\xi_K$ so that the oscillations are just determined by the potential scattering, $\propto\cos(2k_F r-\pi D/2+2\delta_P)-\cos(2k_F r-\pi D/2)$, vanishing if δ_P is also zero. However, at $r\gg\xi_K$, we find that $F(r/\xi_K)\to-1$, which is equivalent to $\delta_P\to\delta_P+\pi/2$. We recover again the potential scattering result, but now the phase shift picks up an additional contribution of $\pi/2$ from the Kondo scattering.

To derive these results, following Ref. 2, it is convenient to relate the scaling function, $F(r/\xi_K)$, to the $\mathcal{T}$ matrix, $\mathcal{T}(\omega)$, which has already been well-studied by a number of methods and is a universal scaling function of ω/T_K. This can be done using the standard formula for the (retarded) electron Green's function,

$$G(\vec{r},\vec{r}\,',\omega)=G_0(\vec{r}-\vec{r}\,',\omega)+G_0(\vec{r},\omega)\mathcal{T}(\omega)G_0(-\vec{r}\,',\omega), \quad (3)$$

where G_0 is the Green's function for the noninteracting case (with $J=V=0$). This result is a direct consequence of the assumed δ-function form of the Kondo (and potential scattering) interaction. The density is obtained from the retarded Green's function by

$$\rho(r)=-\frac{2}{\pi}\int_{-\infty}^{0} d\omega\,\mathrm{Im}\,G(\vec{r},\vec{r},\omega). \quad (4)$$

(The factor of 2 arises from summing over spin.) The exact noninteracting Green's function is

$$G_0=\frac{-ik_F}{v_F\tilde{k}}\left(\frac{-i\tilde{k}}{2\pi r}\right)^{(D-1)/2}\exp(i\tilde{k}r) \quad (D=1,3)$$

$$=-[k_F/(\pi v_F)]K_0(-i\tilde{k}r) \quad (D=2), \quad (5)$$

where $\tilde{k}\equiv\sqrt{k_F^2+2k_F\omega/v_F}$ and $K_0(z)$ is the modified Bessel function. This gives the asymptotic behavior at $r\gg1/k_F$, $\omega\ll\mathcal{D}$,

$$G_0^2(r,\omega)\to-\frac{1}{v_F^2}\left(\frac{-ik_F}{2\pi r}\right)^{D-1}\exp(2ik_F r+2i\omega r/v_F). \quad (6)$$

(This asymptotic behavior holds for general dispersion relations.) The $\mathcal{T}$ matrix in D dimensions can be written at $\omega\ll\mathcal{D}$: $\mathcal{T}(\omega)=t(\omega/T_K,\delta_P)/(2\pi\nu_D)$, where t is a universal dimensionless function of ω/T_K, and ν_D, the density of states per spin at the Fermi energy, has the value $\nu_D=k_F^{D-1}/(c_D v_F)$, with $c_3=2\pi^2$, $c_2=2\pi$, and $c_1=\pi$. Note that $G_0\mathcal{T}G_0$ is proportional to the difference between the s-wave Green's function with and without the Kondo and potential scattering interactions, since the other spherical harmonics are unaffected by the interactions and cancel in $G-G_0$. The effect of the s-wave potential scattering at long distances is just to multiply the s-wave Green's function by the phase $e^{2i\delta_P}$, thus giving

$$t(\omega/T_K,\delta_P)=e^{2i\delta_P}[t_K(\omega/T_K)+i]-i, \quad (7)$$

where $t_K(\omega/T_K)$ is the part of the t matrix coming from the Kondo scattering. Combining Eqs. (3)–(7) gives

$$\rho(r)-\rho_0\to\{c_D/[\pi^2 v_F(2\pi r)^{D-1}]\}\mathrm{Im}\left\{(-i)^{D-1}e^{2ik_F r}\times\int_{-\infty}^{0}d\omega e^{2i\omega r/v_F}\{[t_K(\omega/T_K)+i]e^{2i\delta_P}-i\}\right\}. \quad (8)$$

Essentially this formula (for $D=3$ only) was derived in Ref. 2 except that our treatment of *p-h* symmetry breaking is quite different. Furthermore, we apply more complete knowledge of the $\mathcal{T}$ matrix. We expect this formula to be valid whenever ξ_K, $r\gg1/k_F$, regardless of the ratio r/ξ_K. The function $t_K(\omega/T_K)$ is determined from the *p-h* symmetric Kondo interaction and so it obeys $t_K^*(\omega/T_K)=-t_K(-\omega/T_K)$. Furthermore, $t(\omega/T_K)$ is analytic in the upper half complex ω plane since it is obtained from the retarded Green's function. It then follows that $\int_{-\infty}^0 d\omega\exp(2i\omega r/v_F)t_K(\omega/T_K)$ is purely real. A rescaling of the integration variable implies that we may write

$$\int_{-\infty}^{0}d\omega e^{2i\omega r/v_F}t_K(\omega/T_K)\equiv[v_F/(2r)][F(rT_K/v_F)-1], \quad (9)$$

where the universal scaling function F is purely real. Thus

$$\rho(r)-\rho_0\to\{c_D/[2\pi^2(2\pi)^{D-1}r^D]\}\times\mathrm{Im}\{(-i)^{D-1}e^{2ik_F r}[F(r/\xi_K)e^{2i\delta_P}-1]\}, \quad (10)$$

giving the result announced in Eq. (2). While this derivation assumed that the Kondo interaction is a spatial δ function leading to the simple result, Eq. (3), we expect our asymptotic formula for $\rho(r)$ to be much more generally true, at length scales large compared to the range of the Kondo interaction.

A perturbative calculation of the $\mathcal{T}$ matrix[9] gives

$$t_K(\omega)=-(3i\pi^2/8)[\lambda_0^2+\lambda_0^3\ln(\mathcal{D}/\omega)^2+\cdots], \quad (11)$$

where $\mathcal{D}$ is of order the ultraviolet cutoff. The quantity in brackets can be recognized as the first two terms in the expansion of the square of the running coupling $\lambda^2(\omega)$. For $\omega\gg T_K$, $\lambda(\omega)\to1/\ln(|\omega|/T_K)$, so one expects $t_K\to-3\pi^2 i/[8\ln^2(|\omega|/T_K)]$. Substituting the perturbative expansion into Eq. (9) gives $F(r/\xi_K)=1-(3\pi^2/8)[\lambda_0^2+2\lambda_0^3\ln(r/a)+\cdots]$, where a is a short-distance cutoff of order $v_F/\mathcal{D}$. Again, we recognize the first terms in the expansion of $\lambda^2(r)$, implying the short-distance behavior,

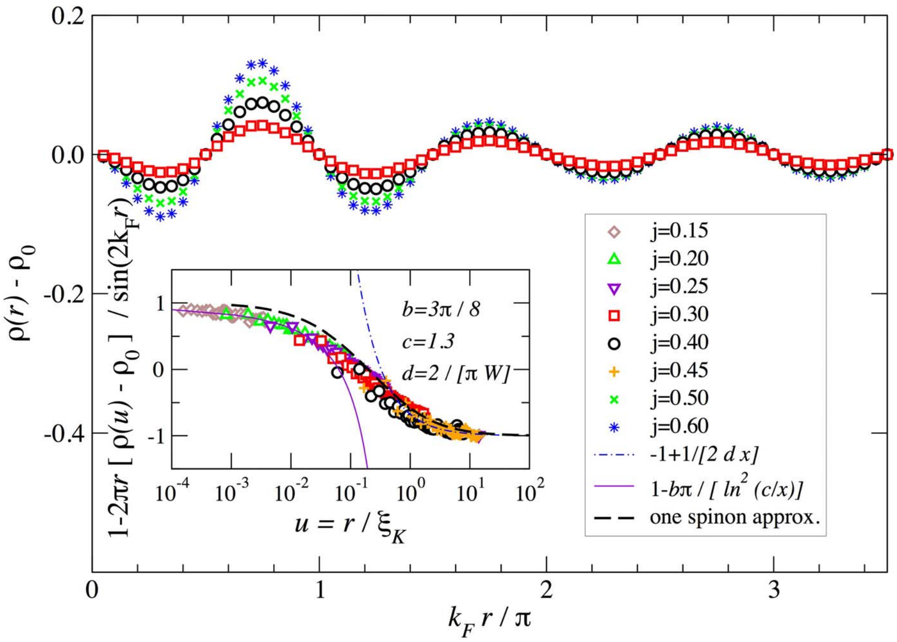

FIG. 1. (Color online) NRG results on charge oscillations around a Kondo impurity coupled to 1D conduction electrons with particle-hole symmetry. Note that the oscillations vanish at $k_F r/\pi \in \mathbb{N}$. As shown in the inset, the properly rescaled envelope function of the oscillations (extracted as $\rho - \rho_0$ at the local maxima) for different Kondo couplings collapses nicely into one universal curve except for the points where $r \sim k_F^{-1}$. In the inset, we show the analytical results for the asymptotics as well: Note the good agreement between the analytical results and the numerics.

$$F(r/\xi_K) \to 1 - 3\pi^2/[8 \ln^2(\xi_K/r)] \quad (r \ll \xi_K). \tag{12}$$

It is an interesting fact that $F(r/\xi_K)$ is apparently given by renormalization-group improved perturbation theory for $r \ll \xi_K$. This is quite unlike the situation for a related quantity, the Knight shift.[4] This is again given by a scaling function, $\chi(r) = (1/T_K) f(r/\xi_K)$ at zero temperature. However, in this case the term of $O(\lambda_0^3)$ has a coefficient that diverges as the temperature $T \to 0$, even at a fixed small r. This means that the Knight shift at short distances $(r \ll \xi_K)$ is *not* given by renormalization-group improved perturbation theory, unlike the Friedel oscillations. Instead, the Knight shift exhibits a nonperturbative behavior, even at short distances. A conjecture was made for this nontrivial short distance behavior in Ref. 4. The fact that $F(r/\xi_K)$ is perturbative at small r/ξ_K seems to follow from the fact that $\mathcal{T}(\omega/T_K)$ is perturbative at large ω/T_K together with Eq. (9), which presumably implies that the short-distance behavior of F is given by the high-frequency behavior of $\mathcal{T}(\omega/T_K)$. The general question of which quantities are perturbative or nonperturbative at short distances in the Kondo model (and other quantum impurity models) remains open.

Perturbation theory for the Friedel oscillations breaks down at r of $O(\xi_K)$ but at $r \gg \xi_K$ we may use Nozières' local Fermi liquid theory. This gives the $\mathcal{T}$ matrix: $t_K \to -i(2 + i\omega/T_B - 3\omega^2/4T_B^2 + \cdots)$. Here T_B corresponds to a particular definition of the Kondo temperature. (See, for example, Chap. 4 of Ref. 1.) It is related to the Wilson definition, called simply T_K in Ref. 1 by $T_B = 2T_K/(\pi w)$ with the Wilson number $w \approx 0.4128$. Substituting in Eq. (9) gives

$$F(r/\xi_K) \to -1 + \pi w \xi_K/(4r) - 3(\pi w)^2 \xi_K^2/(32 r^2) + \cdots \quad (r \gg \xi_K), \tag{13}$$

where we have defined ξ_K precisely in terms of the Wilson definition of T_K: $\xi_K \equiv v_F/T_K$. Nozières' perturbation theory can be turned into a full perturbation theory[10] by taking into account more irrelevant operators in the vicinity of the low-energy fixed point, which give higher-order terms in Eq. (13).

In order to strengthen our analytical results, we have performed extensive numerical renormalization-group (NRG) calculations.[11,12] In Wilson's NRG technique—after a logarithmic discretization of the conduction electron band—one maps the original Kondo Hamiltonian to a semi-infinite chain with the impurity at the end. As a direct consequence of the logarithmic discretization, the hopping amplitude along the chain falls off exponentially. This separation of energy scales allows us to diagonalize the chain Hamiltonian iteratively in order to approximate the ground state and the excitation spectrum of the full chain. If one is interested in spatial correlations, however, some care is needed. The cornerstone of the model, the logarithmic discretization, causes not only the exponential falloff of the hopping amplitude, but also a very poor spatial resolution away from the impurity. To tackle that problem, we introduce Wannier states centered both around the impurity and the point of interest r thus reducing the problem to a two impurity type calculation. Such an approach was demonstrated to work recently by evaluating the spin-spin correlation function around a Kondo impurity; see Ref. 13. To get the amplitude of the charge oscillations, one needs the explicit value of k_F, which we obtained by calibrating the NRG code with a pure potential scattering model.

We show results for different Kondo couplings in Fig. 1. $\rho(r) - \rho_0 \sim \sin(2k_F r)$ in agreement with Eq. (2) for $\delta_P = 0$, the expected p-h symmetric result, since we use a flat symmetric band with no potential scattering. In the inset of Fig. 1, we show NRG results for $F(r/\xi_K)$ showing good agreement with the asymptotic predictions of Eqs. (12) and (13) and fair agreement with the prediction of the "one spinon approximation"[2,14] $t_K = -2i/(1 - i\omega/T_B)$, $F(u) = 1 + 4uae^{2ua}\mathrm{Ei}(-ua)$, $a = T_B/T_K = 2/(\pi w) \approx 1.542$. (Ei is the exponential-integral function.) This is a challenging NRG calculation since universal behavior is only expected to occur for $\xi_K, r \gg k_F^{-1}$ (i.e., at distances beyond several periods of the density oscillation and at weak coupling). On the other hand, the numerical error increases at large r. The nonuniversal, coupling-dependent part of the charge-density oscillations is much more extended in space than that of the spin-spin correlator computed in Ref. 13. That is the main source of the scattering of data points in the inset of Fig. 1. It is interesting to note from the figure that $F \approx 0$, corresponding to the midpoint of the crossover from weak to strong coupling, occurs at $r \approx (0.12 \pm 0.02)\xi_K$. Thus an experimental detection of the Kondo screening cloud via the density oscillations would "only" need to measure out to distances of order $\xi_K/10$ to see at least half of the crossover. In STM experiments, the most readily accessible measure of the Kondo temperature is the half-width of $\mathrm{Im}\,\mathcal{T}(\omega)$, $T_{1/2} \approx 2T_K$.[12] Once this number is determined experimentally, the midpoint of the crossover of the Friedel oscillations is predicted to occur at $r \approx v_F/(5T_{1/2})$. At finite temperature, Friedel oscillations decay exponentially with a thermal correlation length $\xi_T \equiv 2\pi v_F/T$, so it is necessary to be at sufficiently low T that $\xi_K > \xi_T$ to measure the Kondo screening cloud. Direct electron-electron interactions, ignored in the Kondo model, can also lead to decay of the Friedel oscillations with a decay length related to the inelastic-scattering length. However, Fermi liquid theory (typically believed to be valid in $D=2$ or 3) implies that this length also diverges as $T \to 0$.

The Kondo screening cloud *does not* show up in the energy-resolved density of states, $-(2/\pi)\mathrm{Im}\, G(\vec{r},\vec{r},\omega)$, measured in STM and given by Eq. (3). This has a trivial r dependence $1/r^{D-1}$ at $r \gg 1/k_F$. At fixed r, the Kondo scale only enters through the ω dependence. Only after doing the ω integral to get the total electron density does the Kondo scale appear in the r dependence.

Previous attempts[3] to fit experimental data on density oscillations around Cu and Mn impurities in Al to formulas like Eq. (2) have yielded characteristic lengths that are much smaller than ξ_K as determined from the experimentally measured Kondo temperature. We think these issues deserve revisiting, using STM. $\mathrm{Im}\,\mathcal{T}$, measured from the energy-resolved density of states (at a fixed location near the impurity), has a peak with a width identified as T_K. This identification is not completely obvious since it is typically not feasible to raise the temperature past T_K (due to diffusion of the impurity) nor to apply magnetic fields corresponding to Zeeman energies of $O(T_K)$. It follows from Eq. (4) that there should be a change in the envelope of the density oscillations at the corresponding length scale v_F/T_K. An accurate measurement of $\rho(r)$, if it agrees with our results, would both resolve an open fundamental question in Kondo physics and firmly establish that these systems really do exhibit the Kondo effect. We emphasize that the large size of the Kondo cloud makes it very hard to observe. At such large distances that $F(r/\xi_K)$ has changed significantly from its short distance asymptote of 1, the $1/r^D$ factor in Eq. (2) makes the oscillations very small. Clearly the situation is improved in two-dimensional systems.

In conclusion, we have shown that the Friedel oscillations around a Kondo impurity exhibit a universal behavior characterized by the length scale ξ_K. We have determined the corresponding universal scaling function analytically in both limits $r \ll \xi_K$ and $r \gg \xi_K$ and numerically at intermediate r/ξ_K. It exhibits renormalization-group improved weak-coupling behavior at short distances, quite unlike the Knight shift, raising intriguing general questions about which quantities are perturbative and which are not in this limit, for this and other models. The envelope of the oscillations, given in Eq. (2), exhibits a crossover from short to long distances corresponding to an increase of the s-wave phase shift by $\pi/2$. However, at intermediate distances, the result *does not* correspond to simple potential scattering for *any* value of the phase shift. We have determined precisely the distance at which the crossover occurs in terms of the measure of the Kondo temperature accessible to STM experiments.

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