

RKKY interaction and Kondo screening cloud for strongly correlated electrons

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The RKKY law and the Kondo screening cloud around a magnetic impurity are investigated for correlated electrons in one dimension (Luttinger liquid). We find slow algebraic distance dependences, with a crossover between both types of behavior. Monte Carlo simulations have been developed to study this crossover. In the strong-coupling regime, the Knight shift is shown to increase with distance due to correlations. [S0163-1829(96)03447-9]

Since its discovery, the indirect Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction between localized magnetic impurities embedded in a host metal has played an important role in the theory of magnetism. The magnetic moment of one impurity scatters conduction electrons, which are then seen by some other impurity. This second-order process results in the $2k_F$ oscillatory RKKY interaction between different magnetic moments,^{1,2} where k_F is the Fermi momentum. For a lattice of magnetic impurities, this interaction favors magnetically ordered phases determined by the lattice geometry. The RKKY interaction is a basic ingredient for many phenomena in strongly correlated systems, e.g., magnetic impurities in quantum wires,³ normal-state magnetism in high-temperature superconductors,⁴ or magnetic ordering in heavy fermion materials.⁵⁻⁸

For uncorrelated conduction electrons, the RKKY interaction in d dimensions is $\sim \cos[2k_F x]/x^d$, where x is the distance between the localized moments.^{1,2} Within the random-phase approximation or Fermi-liquid theory, this law is not expected to change qualitatively.² At the same time, however, it is known that Coulomb interactions can modify spin- or charge-density correlation exponents in one dimension (1D).⁹⁻¹⁴ In this report, we show that the RKKY interaction indeed exhibits only a slow algebraic decay $\sim \cos[2k_F x]/x^{g_c}$, with an interaction-dependent exponent $g_c < 1$. To examine how the RKKY law is affected by the Kondo effect in such a strongly correlated system, we study the magnetic screening cloud around a single Kondo impurity. We predict the asymptotic behavior far away from the impurity, and discuss qualitatively how RKKY relates to Kondo screening physics in a Luttinger liquid. The crossover between these two regimes has been analyzed by Monte Carlo (MC) simulation.

To describe the low-energy properties of correlated 1D conduction electrons, we employ the bosonization technique.^{9,10} The spin- $\frac{1}{2}$ electron field operator can equivalently be expressed in terms of spin and charge boson fields, which obey the algebra (we put $\hbar = 1$)

$$[\phi_i(x), \theta_j(x')] = -\frac{i}{2} \delta_{ij} \text{sgn}(x-x'), \quad (1)$$

where i and j denote the charge (c) or spin (s) degrees of freedom. The canonical momentum for the θ_i phase field is $\Pi_i(x) = \partial_x \phi_i(x)$. Written in terms of the boson fields, the right- or left-moving component ($p = \pm$) of the electron annihilation operator for spin $\alpha = \pm$ is

$$\psi_{p\alpha}(x) = \frac{1}{\sqrt{2\pi a}} \eta_{p\alpha} \exp[-i\sqrt{\pi/2}[\phi_c(x) + \alpha\phi_s(x)]] \\ \times \exp[ipk_F x + ip\sqrt{\pi/2}[\theta_c(x) + \alpha\theta_s(x)]], \quad (2)$$

where $a = v_F/\omega_c$ is a short-distance cutoff (ω_c is the bandwidth cutoff, say, the Fermi energy, and v_F is the Fermi velocity). The unitary zero-mode operators $\eta_{p\alpha}$ annihilate a particle from branch $p\alpha$, and ensure that anticommutation relations hold between operators with different $p\alpha$.¹⁰ In contrast to models without spin flips, they have to be considered explicitly here to account for all minus signs.

The archetypical low-energy theory for correlated electrons in 1D is the Luttinger liquid model,¹⁰ which unifies the low-temperature physics of microscopic lattice models for strongly correlated fermions. There are only two relevant interaction constants g_c and g_s . The charge interaction constant is $g_c \approx [1 + 2U/\pi v_F]^{-1/2} \leq 1$, where U is the forward-scattering amplitude of the screened Coulomb interaction potential. The Luttinger liquid model assumes that one is away from half-filling, so that umklapp scattering is not present. In addition, electron-electron backscattering processes are neglected, albeit one can incorporate them by a renormalization of the interaction constants or by a perturbative renormalization group (RG) scheme, where the fixed-point value is given by $g_s = 1$.¹² Therefore, we will put $g_s = 1$ in the following to respect the underlying SU(2) spin symmetry of the electrons. The Hamiltonian of the clean system is then given by

$$H_0 = \sum_{j=c,s} \frac{v_j}{2} \int dx [g_j \Pi_j^2 + g_j^{-1} (\partial_x \theta_j)^2], \quad (3)$$

where $v_j = v_F/g_j$ is the velocity of charge- or spin-density waves for the case of full Galilean translational invariance considered here.¹²

Let us now add a spin- $\frac{1}{2}$ magnetic impurity at $x=0$. We use the standard contact term with the conduction electrons, $H_I = J\vec{s}(0)\vec{S}$,^{15,16} where J is the direct exchange coupling, \vec{S} the impurity spin operator, and $\vec{s}(x)$ the spin-density operator, which from Eq. (2) reads, in bosonized form,

$$\begin{aligned} s_z(x) &= \frac{\partial_x \theta_s}{\sqrt{2\pi}} + \frac{\sigma_z}{\pi a} \cos[2k_F x + \sqrt{2\pi} \theta_c(x)] \\ &\quad \times \cos[\sqrt{2\pi} \theta_s(x)], \\ s_{\pm}(x) &= \frac{1}{\pi a} \exp[\pm \sqrt{2\pi} i \phi_s(x)] \\ &\quad \times \{ \pm i \sigma_y \cos[\sqrt{2\pi} \theta_s(x)] + \sigma_x \\ &\quad \times \cos[2k_F x + \sqrt{2\pi} \theta_c(x)] \}, \end{aligned} \quad (4)$$

with $s_{\pm} = s_x \pm i s_y$. Here we have used that $\eta_{p\alpha}$ show up only as bilinear forms, for which a convenient representation can be found in terms of Pauli matrices,

$$\begin{aligned} \eta_{p,\alpha}^{\dagger} \eta_{-p,\alpha} &\rightarrow \alpha \sigma_z, & \eta_{p,\alpha}^{\dagger} \eta_{p,-\alpha} &\rightarrow i \alpha \sigma_y, \\ \eta_{p,\alpha}^{\dagger} \eta_{-p,-\alpha} &\rightarrow \sigma_x. \end{aligned} \quad (5)$$

This replacement gives the correct sign for all possible products of $\eta_{p\alpha}^{\dagger} \eta_{p'\alpha'}$ pairs, allowing for a nonvanishing contribution. Therefore the chosen representation is sufficient for the calculation of correlation functions involving only spin or charge densities.¹⁷

To eliminate an explicit dependence of the interaction part H_I on the ϕ_s field, we perform a standard unitary transformation,¹⁶ $U = \exp[\sqrt{2\pi} i \phi_s(0) S_z]$, such that our final Hamiltonian reads

$$\begin{aligned} U H U^{-1} &= H_0 + \frac{\bar{J}}{\sqrt{2\pi}} S_z \partial_x \theta_s(0) + \frac{J}{\pi a} (\sigma_x S_x \cos[\sqrt{2\pi} \theta_c] \\ &\quad + \sigma_y S_y \cos[\sqrt{2\pi} \theta_s] + \sigma_z S_z \cos[\sqrt{2\pi} \theta_s]) \\ &\quad \times \cos[\sqrt{2\pi} \theta_c]_{x=0}, \end{aligned} \quad (6)$$

where $\bar{J} = J - 2\pi v_F$. The four interaction terms include two forward- and two backward-scattering terms with or without spin flip, respectively. Backward scattering ($\sim \cos[\sqrt{2\pi} \theta_c]$) is responsible for RKKY oscillations, while Kondo screening arises due to spin-flip terms ($\sim S_{x/y}$).

Our subsequent discussion is based on the correlation function $C(x) = \langle s_z(x) S_z \rangle$, where the brackets indicate a thermal average. This function describes the spatial correlation of the electron-spin density with the impurity spin. Another impurity spin located at x would see this correlation, and lowest-order perturbation theory in J constitutes an exact derivation of the RKKY law.² While a quantitative discussion of the complicated interplay between the RKKY interaction and Kondo screening behaviors requires a study of higher-order terms in the corresponding two-impurity model,^{7,8} the main qualitative features of this interplay can already be extracted from $C(x)$.⁷ In this work, we therefore focus on the local screening properties induced in a Luttinger liquid by the presence of a single impurity. A related quan-

tity of direct experimental relevance is the local susceptibility $\chi(x) = \partial \langle s_z(x) \rangle / \partial B$, which was recently reconsidered for the uncorrelated case¹⁸ and is proportional to the Knight shift. Linear-response theory gives ($\beta = 1/k_B T$)

$$\chi(x) = \beta C(x) + \beta \int dx' \langle s_z(x) s_z(x') \rangle, \quad (7)$$

where the second part does not contribute in the perturbative RKKY regime.

Since the slowly varying part of $C(x)$ leads only to sub-leading terms for $x \gg a$,^{18,19} we restrict ourselves to the $2k_F$ part in the following. After the unitary transformation, we obtain

$$C(x) = \frac{\cos[2k_F x]}{2\pi a} \langle \sigma_z \sin[\sqrt{2\pi} \theta_s(x)] \cos[\sqrt{2\pi} \theta_c(x)] \rangle. \quad (8)$$

As can be seen from Eq. (8), there is no phase shift in the $\cos[2k_F x]$ term. This is clear since Eq. (6) does not include elastic potential scattering by the impurity.

The standard treatment of the RKKY interaction² corresponds to a calculation of the correlation function $C(x)$ by lowest-order perturbation theory in the exchange coupling J . The finite-temperature result is ($x \gg a$)

$$\begin{aligned} C(x) &= -\frac{1}{8a} \frac{J}{2\pi v_F} \left(\frac{\beta \omega_c}{\pi} \right)^{-g_c} \cos[2k_F x] \\ &\quad \times \int_0^{\beta d\tau} \prod_{j=c,s} \left| \sin \left[\frac{\pi}{\beta} (\tau + ix/v_j) \right] \right|^{-g_j}. \end{aligned} \quad (9)$$

For $x \ll x_T$, where $x_T = v_F/k_B T$ denotes the thermal length scale, this yields the RKKY law

$$C(x) \sim -\frac{1}{a} \frac{J}{2\pi v_F} \cos[2k_F x] (x/a)^{-g_c}, \quad (10)$$

while for $x \gg x_T$, an exponential decay on the scale x_T is obtained. It is obvious that spin-flip events do not contribute to the perturbative result (9). Therefore, to lowest order in J , one could just as well consider a static impurity, or, equivalently, a pointlike magnetic field acting at $x=0$. The presence of such a field induces $2k_F$ periodic oscillations in the spin density of the electrons, which are then responsible for the RKKY interaction. Thus the range function² describing the decay of the RKKY oscillation amplitude displays only a slow *algebraic* $\sim x^{-g_c}$ law in the low-temperature regime $x \ll x_T$. In the noninteracting case $g_c = 1$, the usual x^{-1} decay is recovered. This modification of the range function might come as a surprise, since the Coulomb interaction does not couple to spin densities. The slower decay is a many-body effect induced by the presence of correlations.

Starting from order J^2 on, spin flips contribute and it becomes mandatory to treat the dynamics of the impurity spin. The most important aspect of the impurity dynamics is the Kondo effect, leading to a screening of the impurity spin by the Luttinger liquid spin density below the Kondo temperature,¹⁵ $T_K \sim J^{2/(1-g_c)}$. Kondo screening of the impurity becomes important for strong couplings J or at low temperatures. For instance, the second-order contribution to $C(x)$ at $x \ll x_T$ is

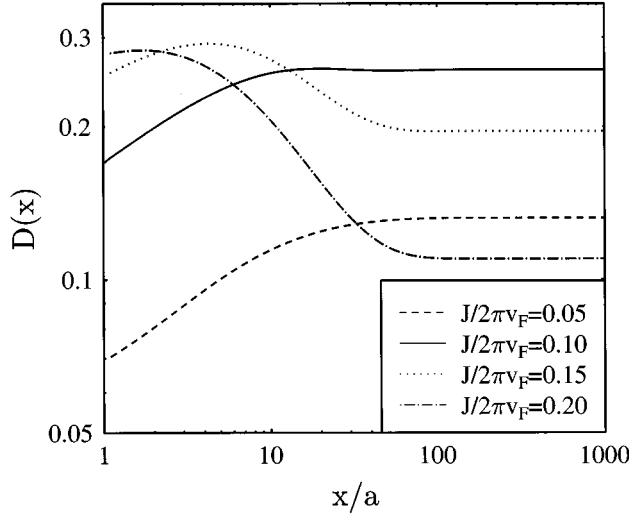


FIG. 1. MC data for $D(x)$ at $g_c = \frac{1}{2}$ and $\beta\omega_c = 100$. Statistical errors are of the order 5%. Notice the logarithmic scales.

$$\delta C(x) \sim -\frac{1}{2\pi a} \left(\frac{J}{2\pi v_F} \right)^2 \cos[2k_F x] (x/a)^{-g_c} \ln(x/a). \quad (11)$$

The logarithmic corrections over Eq. (10) are typical of the Kondo effect, and indicate that we are dealing with a non-perturbative problem.

To study the crossover from the RKKY law to the Kondo screening cloud, we have developed MC simulations. Since the nonlinear terms in Eq. (6) are local, we integrate out all fields away from $x=0$. Under a path-integral representation, we can rewrite $C(x)$ as an average over new fields $q_j(\tau) = \sqrt{2\pi}\theta_j(0, \tau)$, where $j=c, s$, and τ is the Euclidean time, and over the impurity spin field $S(\tau) = 2S_z(\tau) = \pm 1$. The $\sigma_{x,y,z}$ operators have to be treated dynamically as well, but from Eq. (6) it follows that the corresponding field is constrained to be $\sigma_z(\tau) = \mu S(\tau)$ with $\mu = \pm 1$. We find the formal result

$$C(x) = -\frac{1}{2\pi a} \cos[2k_F x] W_c(x) W_s(x) D(x). \quad (12)$$

The functions $W_j(x)$ describe an algebraic decay $\sim x^{-g_j/2}$ on scales $x \ll x_T$, followed by a crossover to an exponential decay,

$$W_j(x) = \left(\frac{\beta\omega_c}{\pi} \sinh \left[\frac{2\pi x}{\beta v_j} \right] \right)^{-g_j/2}. \quad (13)$$

The impurity average is now contained in

$$D(x) = - \left\langle \mu S(\tau=0) \cos \left[\frac{1}{\beta} \sum_{\omega} e^{-|\omega x|/v_c} q_c(\omega) \right] \times \sin \left[\frac{1}{\beta} \sum_{\omega} e^{-|\omega x|/v_F} \left(q_s(\omega) - \frac{\bar{J}}{4v_F} S(\omega) \right) \right] \right\rangle, \quad (14)$$

where the average is taken using the action

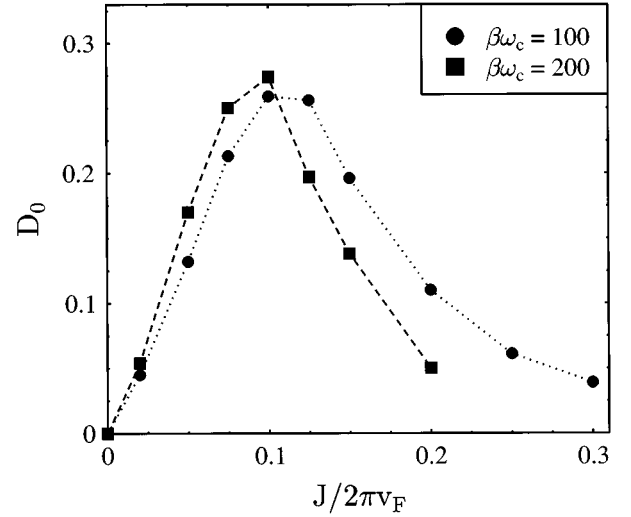


FIG. 2. Numerical results for the plateau value D_0 as a function of J for $g_c = \frac{1}{2}$ and two different temperatures. Statistical errors are of the order of the symbol sizes, and dotted and dashed lines are guides to the eye only.

$$S = \sum_{j=c,s} \sum_{\omega} \frac{|\omega|}{2\pi g_j \beta} |q_j(\omega)|^2 + S_J + \frac{\pi}{2\beta} (\bar{J}/4\pi v_F)^2 \sum_{\omega} |\omega| |S(\omega)|^2. \quad (15)$$

Frequency sums run over Matsubara frequencies, and $q_j(\omega)$ and $S(\omega)$ are the Matsubara components of the respective fields. Discretizing Euclidean time into N slices, $\tau_j = j\Delta\tau$ with $\Delta\tau = \beta/N$, the part S_J becomes

$$e^{-S_J} = \lim_{N \rightarrow \infty} \prod_{i=1}^N \langle \mu S_{i+1}, S_{i+1} | \exp[-\Delta\tau H_J(\tau_j)] | \mu S_i, S_i \rangle, \quad (16)$$

where $H_J(\tau)$ is the last part ($\sim J$) of the Hamiltonian (6), with $\sqrt{2\pi}\theta_{c/s}(0)$ being replaced by $q_{c/s}(\tau)$. The matrix elements can be evaluated in closed form, with σ_z parametrized by μS_i with $S_i = S(\tau_i) = \pm 1$. Since $\exp[-S_J]$ is negative for certain impurity spin paths, our simulation method has to deal with the conventional sign problem.²⁰ Fortunately, the sign problem is moderate except near $T=0$.

In Fig. 1, MC data for $D(x)$ are shown for several J at $g_c = 1/2$. For small J , the function $D(x)$ exhibits a power law $x^{-\delta}$ for $x \ll x_T$, where δ coincides with the RKKY law. Far away from the impurity, $D(x)$ reaches a plateau value D_0 in agreement with Eq. (9). Therefore the RKKY law is fully reproduced by our simulations. For large J , the numerical results display a different behavior. The function $D(x)$ now decreases to a small plateau value, and the RKKY law breaks down even at short length scales. From our numerical data, one has a complete breakdown of RKKY for $J > J^*$ with $J^*/2\pi v_F \approx 0.1$. Furthermore, the numerical simulations predict the asymptotic exponent $(1+g_c)/2$, since $D(x)$ generally reaches its plateau value D_0 for $x < x_T$. From Eqs. (12) and (13), one then infers the asymptotic form of $C(x)$,

$$C(x) \sim \cos[2k_F x] (x/a)^{-(1+g_c)/2}, \quad v_F/T_K \ll x \ll x_T, \quad (17)$$

which we have also verified by using lower simulation temperatures than in Fig. 1.

In view of Fig. 1, it seems convenient to discuss the suppression of RKKY oscillations by Kondo screening in terms of D_0 . Numerical results for the plateau value D_0 at $g_c = \frac{1}{2}$ are shown in Fig. 2. Taking some fixed $J < J^*$ and then going to low temperatures leads to an increase in D_0 . On the other hand, for $J > J^*$, we observe a decrease in D_0 with lower temperatures. This indicates a crossover from a regime $J < J^*$, where RKKY behavior is observed, to a non-RKKY regime $J > J^*$. Finally, for the special value $J = 2\pi v_F$ (Toulouse limit), i.e., $\bar{J} = 0$, one finds the exact result $C(x) = 0$ implying that $D_0 \rightarrow 0$ as J approaches the Toulouse limit. The correlation function $C(x)$ vanishes identically since the Hamiltonian (6) stays invariant under the transformation $\theta_s(x) \rightarrow -\theta_s(x)$, whereas Eq. (8) changes sign.

It is instructive to compare the asymptotic behavior (17) of $C(x)$ with the Friedel oscillation of the charge density. Renormalization group and conformal field theory imply that, in the strong-coupling limit, S_z and $s_z(0)$ form a local singlet.¹⁵ This singlet decouples from the system and simply acts as an elastic potential scatterer in the unitary limit. The Friedel oscillation for that case is given in Ref. 14. In a magnetic field B one obtains, for spin $\sigma = \pm$,

$$\rho_\sigma(x) = \frac{k_F^\sigma}{\pi} - \frac{\sin[2k_F^\sigma x]}{2\pi\alpha_\sigma} (x/\alpha_\sigma)^{-(1+g_c)/2}, \quad (18)$$

where $k_F^\sigma = k_F + \sigma B/4v_F$ and $\alpha_\sigma = 1/2g_c k_F^\sigma$. Clearly, the Friedel oscillation and $C(x)$ are both characterized by the same asymptotic exponent.

As demonstrated in Ref. 18, the Friedel oscillation can also be employed to determine the $T=0$ local susceptibility (7). This quantity is experimentally accessible in terms of the Knight shift. Using $\chi(x) = \partial \langle s_z(x) \rangle / \partial B$ and $\langle s_z(x) \rangle = \sum_\sigma \sigma \rho_\sigma(x)/2$, we obtain the leading asymptotic behavior

$$4\pi v_F \chi(x) = -(x/a_0)^{(1-g_c)/2} \cos[2k_F x] + 1 - \frac{g_c(1-g_c)}{2} \times \sin(2k_F x) (x/a_0)^{-(1+g_c)/2}, \quad (19)$$

where $a_0 = 1/2g_c k_F$. Remarkably, for correlated conduction electrons, the Knight shift actually *increases* with distance. A related behavior has been reported for a nonmagnetic impurity in a Heisenberg chain.²¹

To conclude, for correlated electrons, the RKKY interaction exhibits only a slow algebraic decay. This implies that the usual logarithmic $2k_F$ -singularity of the 1D susceptibility is turned into an algebraic divergence. Furthermore, there is an interesting crossover from RKKY to Kondo screening cloud behavior. Both are characterized by different exponents, and both lead to a slower decay than in the noninteracting case.

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