Anomalous magnetic splitting of the Kondo resonance

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The splitting of the Kondo resonance in the density of states of an Anderson impurity in finite magnetic field is calculated from the exact Bethe-ansatz solution. The result gives an estimate of the electron spectral function for nonzero magnetic field and Kondo temperature, with consequences for transport experiments on quantum dots in the Kondo regime. The strong correlations of the Kondo ground state cause a significant low-temperature reduction of the peak splitting. Explicit formulae are found for the shift and broadening of the Kondo peaks. A likely cause of the problems of large-$N$ approaches to spin-$\frac{1}{2}$ impurities at finite magnetic field is suggested.

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The physics of a magnetic impurity in a metallic host has been studied for many years, and the nature of the ground state and lowest excited states are now understood through the numerical renormalization group (NRG) and the Fermi-liquid theory of the Kondo fixed point. The theoretical situation is much less clear for excitations away from the Fermi surface; however, it is precisely these excitations which are probed by two kinds of current experiments. The nonequilibrium conductance through a quantum dot in a magnetic field $H$, believed to be the clearest sign of Kondo physics in such systems, is determined by the electron spectral function on the dot away from the Fermi energy. The Kondo peak in the spectral function at the Fermi level splits for $H > 0$ into two peaks which move away from the Fermi level with increasing $H$. The subject of this paper is an approximate calculation of this spectral function, based on the exact Bethe-ansatz solution of the $s$-$d$ model.

The differential conductance through a quantum dot at finite bias but $H = 0$ was calculated by Meir, Wingreen, and Lee applying the non-crossing approximation (NCA) to the Anderson Hamiltonian

$$H = \sum_{\sigma,k} \epsilon_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{\sigma} \epsilon_d c_{d,\sigma}^\dagger c_{d,\sigma} + U n_{d,\uparrow} n_{d,\downarrow} + \sum_{\sigma,k} (V_{k,\sigma} c_{k,\sigma}^\dagger c_{d,\sigma} + \text{h.c.})$$

(1)

The NCA is a large-$N$ technique which sums a class of diagrams sufficiently general to resolve the Kondo temperature $T_0$. However, at finite magnetic field the NCA was found to give spurious peaks in the density of states, and thus a perturbative equations-of-motion (EOM) approach was used in which the energy scale $T_0$ does not exist (i.e., is effectively zero). The resulting splitting of the Kondo-like peaks is exactly twice the $s = \frac{1}{2}$ Zeeman splitting. One motivation for this work was to determine whether the strong correlations of the Kondo ground state cause corrections to the peak splitting.

We develop a nonperturbative estimate of the Kondo peak splitting and shape for all values of the ratio $g\mu H / T_0$. The decreased splitting can be pictured as resulting from the oscillation of the impurity spin due to its interaction with the lead electrons (the time scale for this oscillation is $T_0^{-1}$ for $H = 0$).

We use the Bethe-ansatz solution to calculate exactly the density of states for “spinon” excitations, which are the only excitations at energies up to $g\mu H$ from the Fermi level. The density of states for spinon excitations gives an estimate for the electron impurity spectral function. This approximate technique is known at $H = 0$ to give results consistent with Fermi-liquid perturbation theory and the NRG. There are simple limiting forms for the peak location and broadening when $g\mu H \gg T_0$. In this limit the EOM approach of slowly becomes valid as the Kondo energy scale disappears.

The Bethe-ansatz solutions of the $s$-$d$ and Anderson models give exact results for thermodynamic properties such as magnetization and specific heat. Dynamical quantities such as the electron Green’s function on the impurity site in the Anderson model are not known exactly from the Bethe ansatz (or from any other technique) but are required to understand tunneling and other experiments. For example, the Landauer-type formula for nonequilibrium conductance depends on the spectral function $\rho_{d,\sigma}(\omega) = (-1/\pi) \text{Im} G_{d,\sigma}^R(\omega)$ over all energies between the source and drain voltages.

The spectral function can be written as a sum over energy eigenstates

$$\rho_{d,\sigma}(\omega) = \sum_n \left| \langle 0 | c_{d,\sigma}^\dagger | n \rangle \right|^2 \delta(\omega - (E_n - E_0)) + \left| \langle 0 | c_{d,\sigma} | n \rangle \right|^2 \delta(\omega + (E_n - E_0))$$

(2)

At zero magnetic field, an accurate description of the shape of the Kondo peak in $\rho(\omega)$ follows from assuming the matrix elements to be some constant $C$ for all states connected to the ground state by a single spinon (defined
and a peak at energy consists of a Kondo peak near zero energy from spinons, $\Delta = J$ structure in the matrix elements, and because spinons are spectral function at the Fermi level $\rho(\epsilon) = 1/\pi\Delta$, with $\Delta = \pi\rho_0 \sum |V_k|^2$ the bare linewidth.\(^\text{[2]}\)

The DOS in the exact solution of the Anderson model consists of a Kondo peak near zero energy from spinons, and a peak at energy $U$ from “holons” (the simplest excitations in the charge sector). In the Kondo regime, the Anderson model reduces to the s-d model (an impurity spin with interaction term $JS_s \psi(\sigma)\psi$, $\psi$ the conduction electron field) if we are concerned with energies much less than $U$ above the ground state. Hence, to understand the splitting of the Kondo peak for $0 < g\mu H \ll U$, the spin excitations are the relevant ones and the s-d model is appropriate. Mixed-valence behavior requiring a full Anderson model description is expected to begin at $g\mu H \geq (U\Delta)^{1/2}$, which is a very high field for current experiments on quantum dots.

The exact solution of the s-d model contains a trivial charge sector and a spin sector with eigenstates determined in the thermodynamic limit from solutions of linear integral equations.\(^\text{[3]}\) Just as in Fermi liquid theory, a state is labeled by occupation numbers $n(i) = 0, 1$ on the “rapidities” $\lambda_i$ (here the ordered rapidities $\lambda_i < \lambda_{i+1}$ play the role of momenta in the Fermi liquid theory). However one complication from 1D interaction is that the position of rapidities depends on the occupation numbers $n(i)$. In the thermodynamic limit, we can introduce the density of rapidities $D_r(\lambda) = \Delta i/(\lambda + \Delta - \lambda_i)$ to describe their distribution. Now a state can be labeled in terms of a function $\sigma(\lambda) = n[i(\lambda)]D_r(\lambda)$ on the real line (where $i(\lambda)$ is the integer such that $\lambda_i$ is closest to $\lambda$). Thus $\sigma(\lambda)$ can be interpreted as the density of occupied rapidities $\lambda$ in the state. The total energy and magnetization are expressed as weighted integrals of $\sigma$. All rapidities are filled in the ground state, i.e. $n(i) = 1$ or $\sigma(\lambda) = D_r(\lambda)$.

The Bethe-ansatz solution is universal in the limit bandwidth $D \to \infty$, coupling $c = 2J/(1 - 3J^2/4) \to 0$ with $T_0 = D \exp(-\pi/c)$ finite.\(^\text{[3]}\) The Kondo temperature $T_K$ is defined as the halfwidth of the DOS peak at $T = 0$, and is related to Wilson’s $T_K$ by $T_0 = T_K/\omega$, $\omega = \exp(e + 1/4)/\pi^{3/2} = 0.41071 \ldots$, $c$ Euler’s constant.

At zero magnetic field, the energy to add a “hole” at $\lambda_i$ (i.e., to set $n(i(\lambda_i)) = 0$) is $\tan^{-1}(\exp(\pi\lambda_i/c))$, and such a hole has spin $1/2$. In a magnetic field, filling the lowest rapidities with holes lowers energy, i.e. $n(i) = 0$ for rapidities $\lambda_i$ in the interval $(-\infty, B)$, with $\exp(\pi B/c) = \sqrt{e/2\pi(g\mu H/T_0)}$. With $B > -\infty$, there are two types of spinons: hole-like excitations at $\lambda > B$ with $\Delta S = 1/2$ and particle-like excitations at $\lambda < B$ (where $n[i(\lambda)]$ is changed from 0 to 1) with $\Delta S = -1/2$.

The density of states for spinon excitations is $D_s(\epsilon) = D_r(\lambda)(dE/d\lambda)^{-1}$, evaluated at the value of $\lambda$ with $E(\lambda) = \epsilon$. The density of rapidities $D_r$ for the ground state (note that $D_r$ depends on the occupation numbers $n(i)$) was found for nonzero $H$ in the calculation of the impurity magnetization, so all we need is the energy of the spinon excitation at rapidity $\lambda$. The DOS $D_s(\epsilon)$ contains both the impurity contribution and a (constant) conduction electron part, ignored henceforth. The spinon consists of a single $\delta$-function change in the density $\sigma$ (due to the change in the occupation numbers $n(i)$) plus the (regular) backflow (due to the change in $D_r$ caused by the change in $n(i)$). The backflow $\sigma'(x)$ for a $\delta$-function introduced at $\lambda_h > B$ satisfies

$$\sigma'(\lambda) + \int_B^\infty K(\lambda - \lambda_2)\sigma'(\lambda_2) d\lambda_2 = K(\lambda - \lambda_h)$$

with $K(x) = c/\pi(c^2 + \lambda^2)$. With $B = -\infty$ this becomes, in Fourier space, $\sigma'(\rho) = 1/(1 + e^{-|\rho|})$, so the total density change is $\delta(\rho) = \sigma'(\rho) - 1 = -1/(1 + \exp(-c|\rho|))$.

With a magnetic field, $B > -\infty$ and \(^\text{[3]}\) can be solved by the Wiener-Hopf method. The positive backflow $\sigma'(\lambda)$ now includes both particles ($\lambda > B$) and holes ($\lambda < B$). The energy and magnetization of the spinon can be calculated equivalently by summing over particle or hole states. The original hole is dressed by other holes, increasing its interaction energy but also its magnetization. The total change in energy as $\lambda_h \to B^+$ is exactly sufficient to render the excitation gapless.

The backflow for a hole removed at $\lambda_c < B$ satisfies

$$\sigma'(\lambda) + \int_B^\infty K(\lambda - \lambda_2)\sigma'(\lambda_2) d\lambda_2 = -K(\lambda - \lambda_c)$$

The resulting “particle-like” excitation is gapless as $\lambda_c \to B^-$ and connects smoothly to the hole excitation. For $\lambda_c \ll B$, $\sigma'(\lambda) = -K(\lambda - \lambda_c)$ and the total number of holes removed in the backflow is 1.

The Wiener-Hopf technique gives explicit forms for the Fourier transforms of $\phi(\lambda) = \sigma(\lambda + B)\theta(\lambda + B)$. The results involve the kernel factorization

$$K_+(x) = (K_-(x))^{-1} = \frac{(2\pi)^{1/2}}{\Gamma(1/2 + ix)} \times \exp[-ix(1 + i\pi/2 - \log(-x + i\delta))].$$

For a hole excitation ($\lambda_h > B$):

$$\tilde{\phi}_-(\rho) = P \int_0^\infty dt \frac{\tan(ct/2)K_+(ict/2\pi)e^{-(\lambda_h - B)t}}{2\pi K_-(ct/2\pi)(t - ip)}.$$
The total energy for either type of excitation is given by
\[
E(\lambda) = T_0 e^{B/c}(e^{\pi \lambda/c} + \tilde{\phi}_-(i\pi/c)) - g\mu H (1 + \tilde{\phi}_-(0))/2
= g\mu H (\sqrt{e^{2\pi \lambda/c} + \tilde{\phi}_-(i\pi/c)} - 1 + \tilde{\phi}_-(0))/2.
\]

The ground-state density of rapidities \(\sigma_{gs}(\lambda)\) also satisfies an equation of Wiener-Hopf type with source term \(2c/\pi(4\lambda^2 + c^2)\). The solution for \(\sigma_{gs}\) is always peaked near \(\lambda = 0\), with \(\sigma_{gs}(\lambda) = 1/2c\cosh(\pi \lambda/c)\) for \(B/c \ll 0\) and \(\sigma_{gs}(\lambda) = 2c/\pi(4\lambda^2 + c^2)\) for \(B/c \gg 0\). The explicit solution \([2]\) combined with \([3]\) gives the single-spinon density of states. The full (thermodynamic) density of states up to energy \(g\mu H\) is a sum of convolutions of the single-spinon result. The single-spinon density of states at zero energy gives the exact spin susceptibility and specific heat, whose ratio (the Wilson ratio) does not change with magnetic field. \([1]\)

\[\tilde{\phi}_-(0) = 1 - \int_0^\infty dt \frac{\sin(ct)}{\pi K_-(0)t} e^{-(B-\lambda_0)t} K_-(ict/2\pi), \quad \tag{7}\]
\[\tilde{\phi}_-(i\pi/c) = -\int_0^\infty dt \frac{\sin(ct)K_-(ict/2\pi)e^{-(B-\lambda_0)t}}{\pi K_-(i/2)(t - \pi/c)} e^{\pi(B-\lambda_0)/c}. \quad \tag{8}\]

The spectral function estimate for \(g\mu H/T_0 = 48\) (\(B/c = 1.1\)) for comparison to the experimental curve (d) of Goldhaber-Gordon et al. \([16]\) in a field of 7.5 T from \(V_{ds} = -200\mu V\) to 200\(\mu V\) with \(g\mu H/T_0 \approx 50\). (b) is (a) broadened by a temperature \(T = 90\) mK \([16]\) and (c) is the EOM result broadened by the same amount.

The spectral function estimate for spin-up electrons follows from the single-spinon density of states by taking \(\rho_1(\omega) = \frac{1}{2}D_s(|\omega|)\) with \(\sigma = +\frac{1}{2}\) for \(\omega > 0\) and \(\sigma = -\frac{1}{2}\) for \(\omega < 0\), where \(\sigma\) is the spin relative to the ground state. States of spin +1/2 above the ground state can be obtained equivalently by adding a spin-up electron or by subtracting a spin-down electron, so the Kondo part of the spectral function is always symmetric under the combined transformation \(H \to -H, E \to -E\).

The shape of the spectral function is determined by the ratio \(g\mu H/T_0\). Fig. 1 shows the spin-up and total spectral functions for \(g\mu H/T_0 = 48\). The peak in the single-spin spectral function has width \(2T_0\) at zero field and shifts away from the Fermi level and broadens with increasing field (Fig. 2). However, the width of the peak decreases as a fraction of \(g\mu H\). The shift of the peak is always greater than the noninteracting level value \(g\mu H/2\), starting at about two-thirds \(g\mu H\) for small \(g\mu H/T_0\) and rising slowly to \(g\mu H\) as \(g\mu H/T_0 \to \infty\). The effect of temperature on the equilibrium spectral function will be slight until \(T \geq T_0\); the effect of high temperature will be to blur of the Kondo correlations (and hence broaden and shift of the peaks toward the EOM result), but this is a smaller effect experimentally than the nonequilibrium broadening. The behavior of the finite-\(T\) magnetization suggests that the temperature needs to be a few times \(T_0\) for a strong effect.

FIG. 1. The spin-up (top) and total ((a) in bottom) spectral function estimate for \(g\mu H/T_0 = 48\) (\(B/c = 1.1\)). For comparison to the experimental curve (d) of Goldhaber-Gordon et al. \([16]\) in a field of 7.5 T from \(V_{ds} = -200\mu V\) to 200\(\mu V\) with \(g\mu H/T_0 \approx 50\). (b) is (a) broadened by a temperature \(T = 90\) mK \([16]\) and (c) is the EOM result broadened by the same amount.

FIG. 2. The peak shift (top) in units of \(g\mu H\) and broadening (bottom) in units of \(2T_0\), for various values of the ratio \(g\mu H/T_0\). The dotted lines are limiting forms \((12)\) and \((13)\).

The spectral function estimate can be compared to existing measurements of the \(H > 0\) differential conductance through a Kondo impurity. \([15, 17]\) Within the NCA at \(H = 0\), the spectral function for nonzero bias \(V_{ds}\) is essentially two broadened copies of the \(V_{ds} = 0\) spectral function, one shifted up by \(V_{ds}/2\) and one down by \(V_{ds}/2\). \([3]\) Note that \(V_{ds}\) is the applied (drain-source) voltage across the dot, rather than the gate potential. The thermal broadening \((T = 90\) mK\) and additional nonequilibrium broadening in \([14]\) mean that the observed peak is wider than the zero-temperature prediction, but the inward shift of the peak center should still be visible, and in \([15]\] and \([16]\) a smaller splitting than the EOM result of \([3]\) was observed. Fig. 1 shows the agreement of our calculated peak location with that measured in \([13]\) for \(|g| = 0.36\), the value suggested by electron
spin-resonance data on 2DEGs [8] for the 7.5 Tesla field in that experiment. The value \(|g| = 0.30\) required for agreement with the EOM result is less likely. The experimental peaks in Fig. 1 show some nonequilibrium broadening [3], but the parameters needed to estimate this broadening were not measured; convolving the theoretical curve with a Lorentzian of variable width gives a very good fit to experiment.

Because \(g\) in heterostructures is difficult to measure directly, a more convincing experimental demonstration of the splitting could be obtained by varying \(g \mu H / T_0\). In experiment [17] the nonequilibrium broadening is relatively large and may blur the correlations enough that the EOM result becomes applicable.

An asymptotic formula for the peak shape in the limit of large magnetic field can be derived from the large-\(B\) limit of \([8]\) and \(\sigma_{g\nu}(\lambda) \approx 2c/\pi(4\lambda^2 + c^2)\):

\[
E(\lambda) / g \mu H = 1 - \frac{1}{2\pi x} + O(x^{-2} \log(x)), \quad x = B - \lambda. \tag{10}
\]

The result for the peak location in this limit is

\[
4 \max \frac{E}{g \mu H} \approx 1 - \frac{1}{1} + \frac{1}{1 - 2 \log(g \mu H \sqrt{e/T_0 \sqrt{2\pi}})}. \tag{11}
\]

In the large-\(H\) limit the split between spin-up and spin-down peaks in the spectral function is \(2g \mu H\) since spin-up and spin-down peaks each shift by \(g \mu H\). The relative correction in \([11]\) is half that in the impurity magnetization \(M \approx (g \mu H / 2)[1 - 1/\log(g \mu H \sqrt{e/T_0 \sqrt{2\pi}})]\).

The peak width (FWHM) in the limit \(H \gg T_0\) is

\[
\Delta E \approx \frac{g \mu H}{2\pi B^2} = \frac{g \mu H}{4\log^2(g \mu H \sqrt{e/T_0 \sqrt{2\pi}})}. \tag{12}
\]

The narrowness of the peak compared to \(g \mu H\) in the large-\(H\) limit is consistent with the EOM results. [8]

There are two subtleties in the calculation worth mentioning. The above expression for the magnetization gives a value continuously varying from \(\Delta M = 1/2\) for hole-like excitations with \(\lambda \gg B\) to \(\Delta M = 1\) for particle-like excitations with \(\lambda \ll B\). There are not continuous-spin excitations; rather the physical excitation combines a dressed spinon with an infinitesimal shift of the chemical potential for spinons \(B\) to give an integer or half-integer total spin. The same phenomenon of apparently continuous quantum numbers was seen in the charge sector of the asymmetric Anderson model. [8] At nonzero \(H\) and \(T = 0\) there is a small jump in the single-spinon density of states at \(E = g \mu H\). This discontinuity is balanced by the appearance of new types of excitations, so that the total (thermodynamic) density of states is continuous but for a \(\delta\)-function at \(E = g \mu H\) from a state in the same \(SU(2)\) multiplet as the ground state.

We now suggest a reason why large-\(N\) techniques like the NCA give a spurious peak at the Fermi level for finite \(H\). Recall that the impurity orbitals transform under \(SU(N)\) rather than in a high-\(S\) representation of \(SU(2)\). The \(N\) degenerate orbitals split in a generalized magnetic field as follows: \(N/2\) shift up by \(g \mu H / 2\) and \(N/2\) shift down by the same amount. [6] The \(N \to \infty\) magnetization curves for this and other splittings are derived in [6]. The Kondo peak near the origin then arises from transitions between states at the same energy, while the split peaks arise from transitions between states at different energy. Counting the weight of each peak in this argument gives the correct value of the spin susceptibility Wilson ratio, \(N/(N - 1)\). [6] The \(N = 2\) problem is qualitatively different than the \(N \geq 4\) problem since there are no degenerate orbitals after the magnetic field is applied, so it is not surprising that the analytic continuation down to \(N = 2\) gives a false peak at the origin, which is a real peak for \(N \geq 4\). The problem of the conductance through a quantum dot in the Kondo regime is a fine example of the subtle properties of nonequilibrium transport in strongly correlated systems.

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Note added in proof: A preprint by T. Costi (cond-mat/0004037) finds comparable results for \(H \leq T_0\) from an NRG calculation of the spectral function.

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Which representation at general $N$ is selected by the $N = 2$ calculation is in general difficult to determine, but for $N = 2^n$ the appropriate representation is the spinor representation (outer products of Pauli matrices) which splits as described.

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