Kondo resonance in the case of strong Coulomb screening

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The effect of Coulomb screening on the magnetic impurity behavior is analysed. Two types of the behavior corresponding to either integer or fractional occupation numbers of the low lying magnetic level are described. The features in the dependence of the resistivity on the magnetic field specific for these regimes are predicted.

1. MODEL

There is a mechanism of the Coulomb screening of charging of a localized electronic state located inside a conductor, which was first discussed by G. Mahan, P. Nozieres and C. De Dominicis, and by K. D. Schotte and U. Schotte [1]. They demonstrated that the rate of a one-electron jump \( 1/\Gamma \) undergoes exponential renormalization due to both the reconstruction of the Fermi seas and the exchange effect. It was supposed later [2] that the same mechanism pertains to the magnetic impurity behavior. I will examine the effect on the properties of a magnetic impurity by calculating the zero temperature impurity resistivity \( \rho \) as a function of magnetic field \( H \) in two regimes of the impurity behavior. Suggestion of the existence of the two regimes is based on the Bethe Ansatz solution of the model of the resonant level in the spinless case [3]. It confirmed that for either a relatively weak Coulomb interaction or a wide enough conduction band the renorm-group approach extending the perturbation expansion in \( \Gamma \) brings correct results out. At the same time, in the case of a strong exchange effect ensuing from the strong Coulomb interaction the solution becomes non-perturbational in \( \Gamma \) for a level lying low inside the conduction band and predicts its fractional occupation.

Following [2], the impurity with \((2j + 1)\) degenerate localized magnetic state \( d_m, m = -j, ... j \) could be specified by a generalized Anderson model with the Hamiltonian

\[
H = \int_{-D}^{D} d\epsilon \left( \sum_{\gamma} \epsilon c_{\gamma}^{\dagger}(\epsilon) c_{\gamma}(\epsilon) + \sqrt{\Gamma/\pi} \sum_{m} [c_{m}^{\dagger}(\epsilon) d_{m} + d_{m}^{\dagger} c_{m}(\epsilon)] \right) + \\
\sum_{m} \left( \sum_{\gamma} \frac{U_{\gamma}}{2\pi} \int d\epsilon d\epsilon' c_{\gamma}^{\dagger}(\epsilon) c_{\gamma}(\epsilon') + \epsilon_D + mH \right) d_{m}^{\dagger} d_{m} \tag{1}
\]

where the energy of the state \( \epsilon_D \ll -\Gamma, -|H| \) is much lower than the chemical potential \( \mu = 0 \), and the full occupation number \( \sum \hat{n}_m, \hat{n}_m = d_{m}^{\dagger} d_{m} \) is limited to zero or one.
Figure 1: Qualitative dependence of the impurity resistivity $\rho$ on magnetic field $H$ for $\varphi_{sc} = -\pi$ (dashed line), $\varphi_{sc} = 0$ (dotted line), $\varphi_{sc} = -2\pi/3$ (solid line) in the integer occupation regime because of a strong intrasite interaction. The 1D channel states of the continuous spectrum $c_\gamma(\varepsilon), |\varepsilon| < D$ are tunneling for $\gamma = m$, if they are of the same symmetry as the appropriate orbital $d_m$. Otherwise, for $\gamma = i_{sc}$, they only screen the charging of the impurity acquiring the phase shifts the sum of which is $\varphi_{sc} = -\sum_i \text{arctan}(U_i/2)$. The phase shift due to scattering on the constant charge of the impurity in the tunneling channels is $\varphi = -\text{arctan}(U/2), U_m = U$.

Accounting for the screening mechanism in Eq. (1) results in additional phase shifts important for the resistivity calculation and in the modification of the tunneling processes. The contribution to the resistivity is expressed by the phase shifts of the tunneling channels $\delta_m$ as $\rho = (2j + 1)\rho_0/(\sum (\sin \delta_m(H))^{-2})$, where $\rho_0$ is a dimensional constant independent of $H$. To calculate these phase shifts one can generalize Friedel’s Sum Rule to our case $\delta_m = \pi n_m - (\pi + \varphi_{sc}) \sum_{m'} n_{m'}/(2j + 1)$, where the condition of the charge neutrality $\varphi_{sc} + (2j + 1)\varphi = -\pi$ is accounted for. Below I will present results for $j = 1/2$, though both the qualitative predictions and the considerations remain true in the general case.

2. INTEGER OCCUPATION REGIME

In the case of a relatively weak exchange effect (following [3] I suppose $D \gg \Gamma U$) the modification of the tunneling process mainly reduces to an increase of the tunneling half-width by a factor of about $(D/\Gamma)^\beta$, where $\beta$ is expressed by the phase shifts [1]. For the low lying level the full occupation number is close to one and

$$\rho = \frac{2\rho_0}{[\sin(\varphi_{sc}/2 + \pi \Delta n/2)]^{-2} + [\sin(\varphi_{sc}/2 - \pi \Delta n/2)]^{-2}}, \quad \Delta n(H) = n_{1/2} - n_{-1/2}$$

(2)

The magnetization $\Delta n$ is a smooth antisymmetric function of $H$. It varies from -1 to 1 when $H$ are passing from $-H_K$ to $H_K$ ($H_K$ is the Kondo energy). Then Eq.(2) means that two minima of $\rho(H)$ dependence exist (fig.1). They are located at $\pm H_x$, where $\Delta n(H_x) = \varphi_{sc}/\pi$. $H_x$ varies from $\infty$ for $\varphi = 0$ (usual Anderson model) to $H_x = 0$ for $\varphi_{sc} = 0$.

In fact, $\delta_m$ is zero at $H = 0$ for any $j$ if $\varphi_{sc} = 0$. This proves that $\rho$ has a minimum at $H = 0$, instead of a maximum as for $\varphi_{sc} = -\pi$. 

2
3. FRACTIONAL OCCUPATION REGIME

If \( \varphi \) is close to \(-\pi/2 \) \( (\varphi_{sc} \approx 0) \) and \( D \ll \Gamma U \) the behavior of the impurity changes drastically. The Pauli’s principle does not prevent a localized electron from tunneling anymore if all wave functions of the filled part of the conduction band decrease to zero near the location of the localized impurity state due to Coulomb repulsion. Owing to the occurrence of a special symmetry \[3\] the Hamiltonian Eq. (2) allows a Bethe Ansatz solution. Indeed, the artificial two-particle \( S \)-matrices neccessary to construct the collective wave-function \[4\] take the form

\[
\hat{S} = -\frac{\epsilon_1 - \epsilon_2 + 2i\Gamma \hat{P}}{\epsilon_1 - \epsilon_2 - 2i\Gamma}
\]

(3)

where \( \epsilon_1, \epsilon_2 \) are the rapidities of the scattering particles and \( \hat{P} \) permutes their spins. These \( S \)-matrices are unitary and satisfy Yang-Baxter equations. It allows to construct the solution following a standard scheme \[5\]. In this scheme the system is considered to be on the ring of the length \( L \), and the periodic boundary conditions are imposed. This leads to the equations of the spectrum of the system.

\[
e^{i\epsilon_1 L} = (-1)^N \frac{\epsilon_1 + i\Gamma}{\epsilon_1 - i\Gamma} \prod_{j=1}^{N} \frac{\epsilon_1 - \epsilon_j - i2\Gamma}{\epsilon_1 - \epsilon_j + i2\Gamma} \prod_{k=1}^{m} \frac{\epsilon_1 - \xi_k + i\Gamma}{\epsilon_1 + \xi_k - i\Gamma}
\]

(4)

\[
\prod_{j=1}^{N} \frac{\xi_1 - \epsilon_j + i\Gamma}{\xi_1 - \epsilon_j - i\Gamma} = -\prod_{k=1}^{m} \frac{\xi_1 - \xi_k + i2\Gamma}{\xi_1 + \xi_k - i2\Gamma}
\]

where \( \epsilon_1 \) and \( \xi_1 \) are the rapidities of the holons and spinons. Their numbers correspond to the full number of electrons and the number of electrons with turned over spin (spin down), respectively. Minimizing of the energy of the system \( \sum \epsilon_j \) under the condition \( R e \epsilon_j > -D \) one can find \[6\] that all rapidities are real in the ground state. Finally, these equations could be reduced to the equations on the densities of charge \( r_1(\epsilon_1) = 1/(L|\epsilon_{i+1} - \epsilon_i|) \) and spin \( r_2(\xi_k) = 1/(L|\xi_{k+1} - \xi_k|) \) rapidities

\[
\frac{1}{2\pi} + \frac{1}{L\pi} \Phi_2(\epsilon - \epsilon_D) = r_1(\epsilon) + \frac{1}{\pi} \int_D^{\mu_1} d\epsilon' \Phi_1(\epsilon - \epsilon') r_1(\epsilon') - \frac{1}{\pi} \int_{-\pi}^{\mu_2} d\xi \Phi_2(\epsilon - \xi) r_2(\xi)
\]

(5)

\[
\frac{1}{\pi} \int_{-\pi}^{\mu_2} d\xi \Phi_2(\xi - \epsilon) r_1(\epsilon) = r_2(\xi) + \frac{1}{\pi} \int_{-\pi}^{\mu_2} d\xi' \Phi_1(\xi - \xi') r_2(\xi')
\]

(6)

\[
\Phi_n(\epsilon) = \frac{n}{2\Gamma 1 + (ne/2\Gamma)^2}
\]

Here \( \epsilon_D \) differs from \( \epsilon_D \) by a constant due to ambiguity of the logarithm. Both densities consist of the volume and impurity parts \( r_a = r_{a,h} + r_{a,imp} \), which are produced by \( 1/(2\pi) \) and \( 1/(L\pi) \Phi_2(\epsilon - \epsilon_D) \) on the left-hand side of (5), respectively. \( r_{a,h} \) are connected with the electron density \( n_h = N/L = n_{h,1/2} + n_{h,-1/2} \) by

\[
n_h = \int_{-\pi}^{\mu_1} d\epsilon r_{1,h}(\epsilon), \quad n_{h,-1/2} = \int_{-\pi}^{\mu_2} d\xi r_{2,h}(\xi)
\]

(7)

This should be used to define \( \mu_1 \) and \( \mu_2 \). Then the impurity occupation numbers are calculated as

\[
n_{1/2} + n_{-1/2} = \int_{-\pi}^{\mu_1} d\epsilon r_{1,imp}(\epsilon), \quad n_{-1/2} = \int_{-\pi}^{\mu_2} d\xi r_{2,imp}(\xi)
\]

(8)
To describe the behavior of the system in this regime I have solved Eq. (5, 6) in the limit \( \Gamma \to 0 \) when all \( \Phi_n(\epsilon) \) transform into a delta-function. The solution shows that:

\[
\begin{align*}
    r_2 &= r_1/2, r_1(\epsilon) = 1/(3\pi) + 2/3\delta(\epsilon - \epsilon_D) \quad \text{for the spin-degenerate filled states } \epsilon < \mu_2; \\
    r_2 &= r_1(\epsilon) = 1/(4\pi) + 1/2\delta(\epsilon - \epsilon_D) \quad \text{for the spin-non-degenerate filled states } \mu_2 < \epsilon < \mu_1; \\
    r_2 &= 0, r_1(\epsilon) = 1/(2\pi) + \delta(\epsilon - \epsilon_D) \quad \text{for the empty states } \mu_1 < \epsilon.
\end{align*}
\]

These results mean that the level remains spin-degenerate with the fractional occupation number equal to 1/3 for each spin component unless \( \epsilon_D \) becomes greater than \( \mu_2 \). It is spin-non-degenerate with the fractional occupation number equal to 1/2 if \( \mu_2 < \epsilon_D < \mu_1 \). The difference \( \mu_1 - \mu_2 = 2H \) shows that all energy parameters of the level undergo renormalization by a factor equal to the fractional occupation number. Returning to the impurity resistivity one can use its expression in terms of the occupation numbers to conclude that there is no field dependence of the impurity resistivity for low lying level \( \epsilon_D \ll 0 \) unless \( H \) becomes more than \( |\epsilon_D| \).

4. CONCLUSION

It was shown that there is a special behavior of the magnetic level lying low inside the conduction band. It occurs under the condition of resonant Coulomb screening when all filled states of the conduction band, deformed by the Coulomb interaction with a localized electron, become about orthogonal to the state of the electron jumping out from the impurity level. Such a behavior is characterized by the fractional occupation number equal to \( (2j + 1)/(2j + 2) \) for the \( (2j + 1) \) degenerate level \( (1/(2j + 2) \) for each component \). The degeneracy cannot be removed unless the magnetic field \( H \) becomes greater than the energy of the level. This behavior is quite different from the other one typical in the case of a weak Coulomb interaction which develops smoothly under the switching on of the Coulomb screening of the impurity charging. The latter corresponds to an integer occupation number. Its degeneracy is removed by the small magnetic field \( H_K \approx D \exp[-\epsilon_D/\Gamma] \), what leads to a well-known hump in the \( \rho(H) \) dependence located at \( H = 0 \). The width of the hump becomes much less than \( H_K \) if the screening effect is essential.

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