Probing of the Kondo peak by the impurity charge measurement

M. I. Katsnelson*
Institute for Molecules and Materials, Radboud University Nijmegen, Nijmegen 6525 ED, The Netherlands

E. Kogan†
Jack and Pearl Resnick Institute, Physics Department, Bar Ilan University, Ramat Gan 52900, Israel

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We consider the real-time dynamics of the Kondo system after the local probe of the charge state of the magnetic impurity. Using the exactly solvable infinite-degeneracy Anderson model we find explicitly the evolution of the impurity charge after the measurement.

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The Kondo effect discovered originally in connection with the resistivity minimum in dilute magnetic alloys [1] turns out to be one of the most interesting many-body phenomena in condensed matter physics [2]. The localized spin-degenerate level embedded in the sea of conduction electrons may influence the properties of the system in a dramatic way. The key feature of the Kondo effect is the formation of the Kondo, or Abrikosov-Suhl, resonance near the Fermi level [3]. This resonance is of crucial importance for so different fields as the physics of heavy-fermion systems [3, 4] and the electron transport through quantum dots [5, 6]. Direct observations of the Kondo resonance at metal surfaces by the scanning tunneling microscopy method [7] enhances the interest to the problem.

In contrast to our detailed understanding of the equilibrium properties of the Kondo system, much less is known about it's real-time dynamics. The time development of the Kondo effect in quantum dots after the voltage change has been considered in Ref. 8. It was shown in Ref. 9 that the probe of the charge state of magnetic impurity leads to suppression of the Kondo resonance. However, the dynamics of the latter process has not been investigated in detail. In this work we study the evolution of the Kondo system after the measurement of the impurity charge.

We proceed with an exactly solvable large-N_f degenerate Anderson model [10, 11] in the infinite-U limit with the Hamiltonian

$$H = P\left[\sum_{k\nu}[\epsilon_k c^\dagger_{k\nu}c_{k\nu} + \epsilon_f f^\dagger_\nu f_\nu] + \frac{1}{\sqrt{N_f}}\sum_{k\nu}\left(V_k f^\dagger_\nu c_{k\nu} + V^*_k c^\dagger_{k\nu} f_\nu\right)\right]P, \qquad (1)$$

where $c_{k\nu}, f_\nu$ are the Fermi operators for the conduction band and f-electrons correspondingly (we consider the case where the f-level lies in the conduction band), $V/\sqrt{N_f}$ is the hybridization parameter, $\nu = 1, 2, \ldots, N_f$ is the "flavor" index and P is the projection operator into the space with $n_f = \sum_\nu f^\dagger_\nu f_\nu < 2$. We consider the case $N_f \to \infty$. In this limit the ground state is [10, 11]

$$\psi_G = A\left(|\Omega> + \sum_{k\nu}^{\text{occ}} \alpha_k f^\dagger_\nu c_{k\nu}|\Omega>\right), \qquad (2)$$

where $|\Omega>$ is the noninteracting vacuum, i.e. a filled Fermi sea of band electrons with Fermi energy ϵ_F.

The wave-function after we probe charge localized at the f-level depends upon the results of the measurement. If we have found the hole the wave-function directly after the measurement is simply

$$\psi(0) = |\Omega> . \qquad (3)$$

Notice that in the accepted approximation the evolution of the system after the measurement probing hole at the f-level coincides with the model of the initially noninteracting band electrons where we suddenly switched on hybridization with the f-level.

In this limit we have, actually, a single-particle problem with the effective basis $|0>=|\Omega>$ and $|k>= f^\dagger_\nu c_{k\nu}|\Omega>$ [10]. The matrix elements of the Hamiltonian in this basis are

$$\begin{aligned} H|0> &= -\epsilon_f|0> + \sum_{k<k_F} V_k|k> \\ H|k> &= -\epsilon_k|k> + V^*_k|0>, \end{aligned} \qquad (4)$$

describing a discreet level with $E = -\epsilon_f$ embedded into continuum, presented by a band of a finite width with a bottom at $E = -E_F$. It is the finite density of states at the bottom of thus appearing band that is responsible for the formation of logarithmic divergences and, consequently, the Kondo energy scale in the problem.

The wave-function can be presented as

$$\psi(t) = a(t)|f> + \sum_{k<k_F} b(k,t)|k>, \qquad (5)$$

with the initial conditions $a(0) = 1$, $b(k, 0) = 0$. For the amplitude to find electron at the f-level, straightforward algebra gives

$$a(t) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + \epsilon_f - \Sigma(\omega)}. \qquad (6)$$

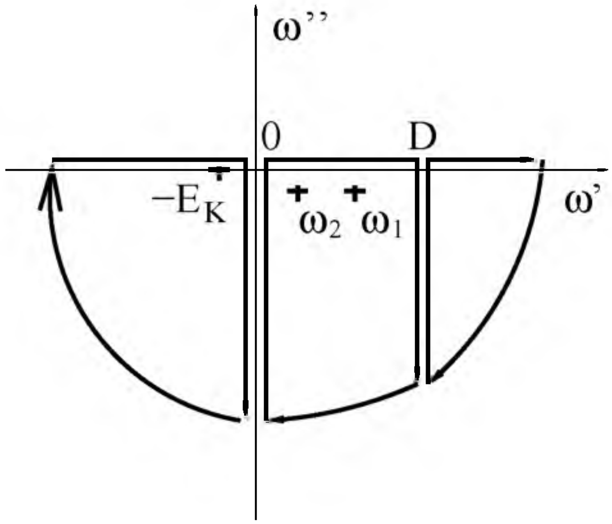

FIG. 1: Contour used to evaluate integral in Eq. (6).

where

$$\Sigma(\omega) = \sum_{k<k_F} \frac{|V_k|^2}{\omega + \epsilon_k}. \tag{7}$$

The transition from the discrete level in the electron band is done by shifting integration contour by an infinitesimal value $+is$. Thus instead of N poles at the real axis, corresponding to discrete electron levels we obtain two branch points: bottom of the band $\omega = D$ and the Fermi energy $\omega = E_F = 0$.

In Eq.(6) the integration contour can be closed in the lower half-plane, so the integral is determined by the singularities of the integrand in that half-plane. We can take the cuts along the line $\omega = -iy$, $\infty > y > 0$ and $\omega = D - iy$, $\infty > y > 0$. Thus

$$a(t) = \sum_{poles,j} e^{-i\omega_j t} R_j + I_{cut}, \tag{8}$$

where j labels the poles of the function $(\omega + \epsilon_f - \Sigma(\omega))^{-1}$ given by the solutions of the equation

$$\omega_j = -\epsilon_f + \sum_{k<k_F} \frac{|V_k|^2}{\omega_j + \epsilon_k + is}, \tag{9}$$

and the corresponding residues are

$$R_j = \left[1 + \sum_{k<k_F} \alpha_k(\omega_j)\right]^{-1}, \tag{10}$$

where $\alpha_k(\omega) = V_k^*/(\omega + \epsilon_k)$. Notice, that for large t only the contribution of the real pole $\omega = -E_K$ survives, to give

$$a(t) = \left[1 + \sum_{k<k_F} |\alpha_k(-E_K)|^2\right]^{-1} e^{iE_K t}. \tag{11}$$

Now we present an alternative point of view at the process of tunneling into continuum, which will clarify the meaning of Eq. (6) and, especially, of Eq. (11). The eigenstates of the Hamiltonian (4) can be easily found:

$$\psi_E = \frac{|0> + \alpha_k(E)|k>}{\sqrt{1 + \sum_{k<k_F} |\alpha_k(E)|^2}}, \tag{12}$$

and the relevant energies are the solutions of the equation

$$E = -\epsilon_f + \sum_{k<k_F} \frac{|V_k|^2}{E + \epsilon_k}. \tag{13}$$

Equation (13) being superficially similar to Eq. (9) is totally different. The former has only real solutions, their number beings equal to the number of electron states below the Fermi level plus one, the latter gives three poles (see below), two of which are complex, and the third real coincides with the ground state energy $E = -E_K$. Notice that in the ground state the f-level hole occupation number is

$$\bar{n}_f = \left[1 + \sum_{k<k_F} |\alpha_k|^2(-E_K)\right]^{-1} = 1 - n_f. \tag{14}$$

The wave-function right after the measurement can be presented as

$$\psi(0) = \sum_E \left[1 + \sum_{k<k_F} |\alpha_k(E)|^2\right]^{-1/2} \psi_E. \tag{15}$$

Hence at any moment t after the measurement the wave-function is

$$\psi(t) = \sum_E \left[1 + \sum_{k<k_F} |\alpha_k(E)|^2\right]^{-1/2} \psi_E e^{-iEt}, \tag{16}$$

and the amplitude to find a hole at the level f is

$$a(t) = \sum_E \left[1 + \sum_{k<k_F} |\alpha_k(E)|^2\right]^{-1} e^{-iEt}, \tag{17}$$

which exactly corresponds to the integral from Eq. (6), calculated by the residues method. For $t \to \infty$ due to dephasing of the contributions from all the states save the bound state we obtain

$$a(t) = \bar{n}_f e^{iE_K t}, \tag{18}$$

coinciding with Eq. (11).

For a more detailed analysis of Eq. (8) we additionally specify our model, assuming $V_k = V = \text{const}$ and flat-band density of bare itinerant-electron states $\rho = \rho_0$. In this model we get

$$\Sigma(\omega) = \Delta \ln\left(\frac{\omega}{\omega - D}\right), \tag{19}$$

where $\Delta = |V|^2\rho_0$; the imaginary part of the logarithm is equal to $-\pi$ at the real axis between the branch points to agree with Eq.(7) at the real axis. In this case there exist two complex poles.

Eq.(8) being valid independently of the strength of the hybridization, we however limit our analysis to the Kondo regime $\Delta \ll -\epsilon_f$, where we get

$$\begin{aligned} E_K &= De^{-|\epsilon_f|/\Delta} \\ \bar{n}_f &= \frac{E_K}{\Delta} \ll 1. \end{aligned} \tag{20}$$

One complex pole $\omega_1 = E_f = -\epsilon_f - i\pi\Delta$, with the residue approximately equal to 1, is responsible for the traditional "Fermi golden rule" decay processes. The second pole $\omega_2 = E_K - i\pi\Delta$ with the residue equal to $-\bar{n}_f$ is the complex "mirror" of the Kondo pole. As can be shown, in the regime we consider, the contribution from the cuts is negligible for small and large t. We may hope the at the semi-quantitative level it can be neglected at all t, though, strictly speaking, the last claim should be substantiated by numerical calculations. Thus

$$a(t) = \bar{n}_f \left(e^{iE_Kt} - e^{-iE_Kt-\pi\Delta t}\right) + e^{i\epsilon_f t - \pi\Delta t}. \tag{21}$$

Due to an entanglement between the localized electron and the Fermi sea the local probe of the former should create the "decoherence wave" [12] in the conduction electron subsystem which will disturb the spin and charge distribution in the latter. Let us calculate the distribution of conduction electrons around the impurity after the measurement. The probability density to find the hole at a distance r from the impurity is given by the expression

$$\rho_c(r,t) = \left|\sum_{k<k_F} V_k e^{ikr}\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega}{\omega+\epsilon_k}\frac{e^{-i\omega t}}{\Sigma(\omega)-\omega-\epsilon_f}\right|^2 \tag{22}$$

The asymptotic of Eq.(22) for large t is obvious: the main contribution comes from the real pole $\omega = -E_K$, and we obtain

$$\rho_c(r) = \left|\bar{n}_f\sum_k \frac{V_k e^{ikr}}{E_K-\epsilon_k}\right|^2. \tag{23}$$

Notice that the coordinate dependence of the hole density of states long after the measurement is the same as in the ground state; only the coefficient is smaller by additional factor $\bar{n}_f$ which is just the suppression factor for the spectral weight of the Kondo resonance [9].

If there exists intermediate asymptotic of exponential decay of $a(t)$, it is described by the complex pole E_f. For these values of time the probability density is determined by the virtually bound state

$$\rho_c(r,t) \sim \left|\sum_k \frac{V_k e^{ikr}}{E_f-\epsilon_k}\right|^2 e^{-2\pi\Delta t}. \tag{24}$$

This asymptotic holds for $\bar{n}_f \ll e^{-\pi\Delta t} \ll 1$.

Assuming for simplicity an isotropic hybridization V and the dispersion law, we can fulfill angular integration in Eqs.(23) and (24). In the perturbative regime we consider, E_K is very close to E_F. Due to the logarithmic divergence of the integral in Eq.(23) the main contribution comes from the vicinity of the upper limit, and we obtain

$$\rho_c(r) = \frac{\sin^2(k_F r)}{(k_F r)^2}\bar{n}_f^2\left(\frac{E_K-\epsilon_f}{V_{k_F}}\right)^2. \tag{25}$$

Now we consider another measurement result. Let the first measurement has found the localized electron sitting at the f-level. The wave-function directly after such measurement according to the von Neumann "wave-function collapse" postulate [13] is again given by Eq. (5) with the initial condition

$$\psi(0) \sim \frac{1}{\sqrt{N}}\sum_{k\nu}^{occ}\alpha_k f_\nu^\dagger c_{k\nu}|\Omega>. \tag{26}$$

After simple algebra we obtain

$$a(t) = \frac{C}{2\pi i}\int_{-\infty}^{\infty} d\omega\frac{e^{-i\omega t}}{\Sigma(\omega)-\omega-\epsilon_f}Y(\omega), \tag{27}$$

where

$$Y(\omega) = -\sum_k \frac{|V_k|^2}{(\omega+\epsilon_k+is)(E_K-\epsilon_k)}. \tag{28}$$

Again closing the contour of the integration and ignoring the contribution from the branch cuts we find (in the perturbative regime)

$$\begin{aligned} a(t) &= \sqrt{\frac{\bar{n}_f}{1-\bar{n}_f}}\left[(1-\bar{n}_f)e^{iE_Kt}\right. \\ &\left.+\bar{n}_f Y(-E_K)e^{-iE_Kt-\pi\Delta t} + Y(\epsilon_f)e^{i\epsilon_f t-\pi\Delta t}\right]. \end{aligned} \tag{29}$$

¿From the orthogonality of eigen-functions corresponding to $-E_K$ or ϵ_f to the wave-function corresponding to E_K we obtain

$$Y(-E_K) = Y(\epsilon_f) = -1. \tag{30}$$

Finally, in the Kondo regime ($\bar{n}_f \ll 1$) one has

$$a(t) = \sqrt{\bar{n}_f}\left[e^{iE_Kt} - e^{i\epsilon_f t-\pi\Delta t}\right]. \tag{31}$$

Thus for $t \to \infty$

$$a(t) = \sqrt{\bar{n}_f}e^{iE_Kt}. \tag{32}$$

This result can be understood in a simple way. Since in the limit under consideration $\Delta \ll -\epsilon_f$ the (hole) occupation number of the f-level is very small, the measurement with the result $\bar{n}_f = 0$ produces negligible disturbance of the wave-function of the ground state. This is in sharp contrast with the measurement which results in $n_f = 1$. After that measurement, as we can see from Eq.(11), the asymptotic value of n_f changes drastically.

We have analyzed two kinds of processes. The process of measurement instantly reduces the ground-state wave function, with the probability to find a hole at the f-level equal to $\bar{n}_f$) to the form (3), with the probability to find a hole at the f-level equal to 1 (we'll consider here only one possible measurement result). After the measurements starts the process of quantum evolution with the characteristic time scale $1/\Delta$, which ends up in the state with the probability to find a hole at the f-level equal to $\bar{n}_f^2$. Notice that we obtained seemingly paradoxical result. On the physical grounds one should expect the disappearance of the measurement effects at large times, and hence the return of the hole-occupation number to $\bar{n}_f$. The way to solve the paradox is clear when we look at Eq. (16). Together with the evolution described by this equation there exists a third kind of a processes: thermalisation of the hole as the result of the excitation of electron-hole pairs. The consideration of such processes demands considering instead of the model $N_f \to \infty$ the model with large but finite N_f and taking into account terms of the order of $1/N_f$. This will be the subject of a separate publication, but already now we can say that in such model the time scale of this thermalisation will be much larger than the time-scales of the evolution described by Eq. (21) and determined by the inverse Kondo temperature. Thus even in such model, our results, say Eq. (18) will be still valid, only it will present an intermediate asymptotic. Notice that what is said in the conclusion is the time-representation of the phenomenon of the density of states description of the Kondo resonance. Whereas in the infinite-N_f limit investigated by us the Kondo peak has a zero width, for finite N_f it is a Lorentzian with both the distance from the Fermi energy and the width of order of the Kondo temperature (and for purely spin case $N_f = 2$ the center of the resonance just coincides with the Fermi energy) [3, 11].

To conclude, we have presented the analytical solution of the problem of real time charge dynamics in quantum impurity system for the exactly solvable infinite-N_f limit. This limit is sufficient to describe the effects of decoherence on the Kondo resonance. On the other hand, the process of recoherence, that is, return to the ground state after the measurement, requires the consideration of the higher-order processes in $1/N_f$.

* Electronic address: M.Katsnelson@science.ru.nl
† Electronic address: kogan@quantum.ph.biu.ac.il

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