Kondo Temperature for the Two-Channel Kondo Models of Tunneling Centers

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The possibility for a two-channel Kondo (2CK) non Fermi liquid state to appear in a metal as a result of the interaction between electrons and movable structural defects is revisited. As usual, the defect is modeled by a heavy particle moving in an almost symmetric double-well potential (DWP). Taking into account only the two lowest states in DWP is known to lead to a Kondo-like Hamiltonian with rather low Kondo temperature, $T_K$. We prove that, in contrast to previous believes, the contribution of higher excited states in DWP does not enhance $T_K$. On the contrary, $T_K$ is reduced by three orders of magnitude as compared with the two-level model: the prefactor in $T_K$ is determined by the spacing between the second and the third levels in DWP rather than by the electron Fermi energy. Moreover, $T_K$ turns out to be parametrically smaller than the splitting between the two lowest levels. Therefore, there is no microscopic model of movable defects which may justify non-Fermi liquid 2CK phenomenology.

It is well known that two-level systems (TLS) determine the low energy phenomena in a glassy matter. The most popular realization of the TLS is a movable atom tunneling between two minima of the two-well potential created by other atoms \cite{1}. The low-temperature behavior of glasses was found to be consistent with the assumption of homogeneous distribution of both energy difference and spatial distance $a$ between the minima. In metallic glasses TLS interact with itinerant electrons. Usually this interaction in metallic glasses is assumed to be weak and to manifest itself only in a finite relaxation rate of the TLS, see Ref. \cite{2} for a review.

It was proposed long ago \cite{3,5} that a TLS interacting with itinerant electrons behaves like a localized spin in the Kondo model. Indeed, in the limit $k_F a \ll 1$, where $k_F$ is the Fermi wavelength, only the electrons with two spherical harmonics, namely, $l = 0$ and $l = 1, m = 0$ interact with TLS. (Here and below the axis of the momentum quantization is the easy axis of TLS, $x$)

Let us introduce a pseudospin $\hat{S}$ of a symmetric TLS: $S = -1/2$ corresponds to the ground state (even wave function), whereas $S = 1/2$ labels the excited state with the odd wave function. One can map the electrons with the two relevant spherical harmonics on the one-dimensional Fermi gas of particles that are characterized by a pseudo-spin with components $\sigma = +, -$ as $\Psi_{l=0} \equiv \Psi_-$, $\Psi_{l=1, m=0} \equiv \Psi_+$, while the real electron spin index $s = \uparrow, \downarrow$ is replaced with the channel index $\mu = 0, 1$. Furthermore, provided that the Fermi energy, $\varepsilon_F$, exceeds all of the relevant energies, one can linearize the electron dispersion law near the Fermi level, $\varepsilon(p) \approx v_F |p|$, where $v_F$ is the Fermi velocity. The divergences caused by the linearized spectrum should, thus, be cut off by the bandwidth $D \simeq \varepsilon_F$. The resulting Hamiltonian of the system can be expressed as

$$\hat{H} = -i v_F \int_{-\infty}^{\infty} dx \sum_{\mu=0,1} \sum_{\sigma=\pm} \Psi_{\mu,\sigma} \partial_x \Psi_{\mu,\sigma} + \sum_{i=x,z} \Delta_i \hat{S}_i + 2\pi i v_F \sum_{j=x,y,z} \sum_{\mu=0,1} \sum_{\sigma,\sigma'=\pm} v_j \Psi_{\mu,\sigma}^\dagger \sigma\sigma' \Psi_{\mu,\sigma'} \hat{S}_j. \quad (1)$$

Here the Pauli matrices, $\gamma_{\sigma\sigma'}$, act in the space of the electron pseudospin, and $\hat{S}$ is the operator of the TLS pseudospin, $[\hat{S}_i, \hat{S}_j^\dagger] = i e^{ij} \hat{S}_k$. The first term in Eq. (1) describes kinetic energies of 1D electrons. The second term characterizes the TLS level splitting: $\Delta_z$ and $\Delta_x$ represent correspondently the tunneling and the initial TLS asymmetry. The third term in Eq. (1) describes TLS-electron interaction. The Hamiltonian Eq. (1) is nothing but the two-channel Kondo Hamiltonian \cite{6}, where the level splitting plays the role of the Zeeman splitting of states of the usual Kondo impurity. For a comprehensive review of implication of this model to magnetic ions and tunneling centers in metals see Ref. \cite{7}.

The two-channel Kondo effect is known to manifest itself through a non-Fermi liquid behavior of the specific heat, magnetization and electronic correlation functions. Such a behavior takes place when both the temperature, $T$, and the level splitting,

$$\Delta = \sqrt{\Delta_z^2 + \Delta_x^2}, \quad (2)$$

do not exceed the Kondo temperature, $T_K$. It can be shown \cite{8} that in the limit $v_z \ll v_x \ll 1$ 

$$T_K = D (v_x v_z)^{1/2} \left( \frac{v_z}{4v_x} \right)^{1/4} \quad (3)$$

The non-Fermi liquid behavior of the TLS at the two-channel Kondo fixed point was used in Ref. \cite{11} to interpret the zero bias anomaly in characteristics of point contacts \cite{12} and more recently \cite{13} to explain the temperature behavior of the dephasing rate observed in
In general, TLS were assumed to play important role in crystalline metals as well as in metallic glasses.

Assumptions of Ref. [12] were criticized on the grounds that the disorder induced splitting estimates were too high for the Kondo-like behavior to develop [13]. Although several questions raised in Refs. [13] remain unanswered, we put this issue aside. Instead, we concentrate on a different objection - smallness of $T_K$ in Eq. (1) for reasonable values of parameters. Here we prove that $T_K \ll \Delta_t$ for any set of the microscopic parameters, which allows the Kondo like description, Eq. (1). Therefore, the two channel Kondo fixed point by no means can be reached with the lowering $T$ and thus is irrelevant for the description of the TLS in metals.

To understand why the resulting Kondo temperature is so small, let us first discuss the physical meaning of the bare coupling constants $v_1$ and estimate them.

The coupling constant $v_1$ in Eq. (1) determines the renormalization of the TLS asymmetry by the electrons - a tilting of the double-well potential by the dipole moment of the electron density. Assuming a contact interaction characterized by a dimensionless coupling constant $\lambda < 1$ we can estimate $v_1$ at given Fermi wave number, $k_F$, and the size of TLS, $a$, as (see, e.g., [2]) $v_1 \propto \lambda k_F a$.

As to $v_2$, it characterizes transition between the two states of the TLS assisted by an electron transition. Incoming electron renormalizes the barrier’s height, $V$, and consequently the tunneling amplitude. However, the tunneling event still has to occur. Therefore, $v_2 \propto \lambda k^2_F a^2 \exp(-\eta)$, where the tunneling exponent $\eta$ is determined by $V$ and the atomic mass $M$. Since $M$ is large, $\eta \gg 1$ even for relatively low barriers. As a result, the coupling constant $v_2$ is always much smaller than $v_1$:

$$v_2 \approx v_1(k_F a) \exp(-\eta) \ll v_1, \quad \eta \approx \hbar^{-1} a \sqrt{8MV}$$

This is why $v_2$ was usually neglected in previous treatments of TLS. For “typical” values of the parameters

$$D \sim 5eV, \quad v_1 \simeq 0.2, \quad v_2/v_1 \simeq 10^{-3},$$

the “conventional” estimate of the Kondo temperature is $T_K \simeq 10^{-2} - 10^{-3} K$ [14]. This low value of $T_K$ makes it hard to believe that the Kondo fixed point is relevant for the discussion of existing experiments.

In attempt to resolve the problem of small $T_K$ authors of Ref. [13] went beyond the two level approximation and considered virtual tunneling through the third level of the “TLS”. This contribution to $v_1$ apparently does not contain the tunneling exponent. According to Ref. [13], this fact dramatically increases $T_K$ comparing to the “conventional” estimate. In our opinion the statement about the large increase in the Kondo temperature is incorrect. Below we discuss the problem in detail.

$T_K$ can be extracted from second order perturbation theory in the interaction of the tunneling particle with the electrons. We calculate this correction within the one-dimensional (1D) model suggested in Ref. [13].

Consider a heavy particle in a symmetric 1D double-well potential $V(x)$. Let the energies of the two lowest eigenstates, $E_{1,2}$, be indistinguishable: $E_2 - E_1 \to 0$. One can express the matrix element of the contact interaction of this particle with electrons through the coupling constant, $\lambda$, Fermi velocity, $v_F$, the heavy-particle eigenfunctions, $\phi_i(x)$, and the electron wave functions, $\psi_\sigma(x)$, with a given isospin, $\sigma = +, -$:

$$U_{ij}^{\sigma_1 \sigma_2} = 2\pi v_F \lambda I_{ij}^{\sigma_1 \sigma_2}, \quad I_{kl}^{\sigma_\rho} \equiv \int dx \phi_k \phi_l \psi_\sigma \psi_\rho.$$ (6)

There are two second order corrections to the scattering amplitude $\sigma_1, i \to \sigma_2, j$, which correspond to processes with different intermediate states:

(i) In the intermediate state an electron has an isospin $\sigma$ and the particle occupies a state $k$ with the energy $E_k \equiv E_1 + \varepsilon_k$ (see Fig. 1a).

(ii) The transition $i \to k$ of the heavy particle produces an electron-hole pair - an electron in the final state $\sigma_2$ and a hole in the state $\sigma$. Afterwards the hole annihilates the electron in the initial state $\sigma_1$ and the heavy particle changes its state from $k$ to the final state $j$ (Fig. 1b).

Combining the contributions of these two processes and taking into account the occupation numbers of electron states at a given temperature $T$ we present the second order correction to the matrix element as:

$$\delta U_{ij}^{\sigma_1 \sigma_2} \propto \lambda^2 v_F^2 \sum_{k,\rho} \int \frac{d\xi}{-T} \left| I_{ik}^{\rho} - I_{jk}^{\rho} \right| \left( 1 + \exp \left( \frac{-\xi}{T} \right) \right). \quad (7)$$

Here $I_{kl}^{\rho}$ is determined by Eq. (3), $\xi$ denotes the energy of the intermediate electron or hole state counted from the Fermi level, and $\varepsilon_k \equiv E_k - E_1$ is the energy of the $k$-th state in the double-well potential counted from its ground state $E_1 = E_2$. We have already discussed that the domain of the integration over $\xi$ should be $|\xi| < D \sim \varepsilon_F$. As to the singularity at $\xi = -\varepsilon_k$, the integral in Eq. (7) should be understood as the principal value. The minus sign in front of the second (hole) term in the numerator is due to the anti-commutation of fermionic operators.

Consider now matrix elements $U_{ij}^{\sigma_1 \sigma_2} = -U_{ji}^{\sigma_2 \sigma_1}$ that describe transitions of the heavy particle between its two lowest states. Using Eqs. (7) one can show that such a transition should be accompanied by the change of the electron isospin: due to the parities of the wave functions...
$U_{12}^- = U_{12}^+ = 0$. To evaluate $U_{12}^-$ we sum over $\sigma$ and integrate over $\xi$ in Eqs. (7). The result can be written as

$$\frac{\delta U_{12}^-}{U_{12}^+} = \lambda u_{\infty}, \quad u_n = \frac{1}{I_{12}} \sum_{k=1}^{n} \sum_{i,j=1}^{2} \epsilon_{ij}^{k} \ln \left( \frac{D}{\varepsilon_{k}} \right), \quad (8)$$

where $\epsilon_{11} = \epsilon_{22} = 0$, $\epsilon_{12}^2 = -\epsilon_{21}^2 = 1$, and

$$c_{ij}^k \equiv I_{ik}^+(I_{jk}^- - I_{jk}^+), \quad \varepsilon_{k}^* \equiv \max \{\varepsilon_{k}, T\}. \quad (9)$$

We start with the contribution of the first two levels ($k = 1, 2$) to the sum over $k$ in Eq. (8). Using Eqs. (7), and (4) one obtains, cf. with Ref. [4],

$$u_2 = \ln \left( \frac{D}{T} \right) \int dx \left[ \phi_2^2 - \phi_1^2 \right] \left( \psi_2^2 - \psi_1^2 \right), \quad (10)$$

The electron wave functions $\psi_{\sigma}(x)$ are standing waves, $\psi_{-}(x) + i\psi_{+}(x) = \sqrt{2} \exp(ik_{F}x)$. Since $k_{F}a \ll 1$ (otherwise this 1D approach is not applicable)

$$\psi_{-}(x) \simeq \sqrt{2} \left[ 1 - (k_{F}x)^2/2 \right], \quad \psi_{+}(x) \simeq \sqrt{2}k_{F}x. \quad (11)$$

We introduce the wave functions, $\phi_{1}(x)$, localized in the left (right) well, $\sqrt{2}\delta\phi_{1} = \psi_{1} = \psi_{2}$, recall that the functions $\phi_{1}$ are normalized, and rewrite Eq. (4) as

$$u_2 = 8 \ln \left( \frac{D}{T} \right) \int dx \left( k_{F}x \right)^{2} \phi_{1}(x)\phi_{2}(x). \quad (12)$$

The wave functions $\phi_{1}(x)$ and $\phi_{2}(x)$ are localized in the different wells, their overlap being exponentially small. Accordingly, $u_2$ is exponentially small as well, and one arrives at the “conventional” estimate for $T_{K}$.

It turns out that taking into account the higher excited states in the double-well potential, i.e., terms with $k > 2$ in the sum Eq. (3), can only reduce the estimation of $T_{K}$.

Indeed, it follows from the definition of $I_{ij}^{\sigma}$, Eq. (3), and completeness of the set of the functions, $\{\phi_{k}\}$, $(\sum_{k} I_{ik}^{\sigma} \phi_{k}(y) = \delta(x - y))$ that the sums, $\sum_{\sigma} I_{ij}^{\sigma}, \sum_{\sigma} I_{ij}^{\sigma} I_{jk}^{\sigma}$ with any set $\sigma$, and consequently $\sum_{k} c_{ij}^{k}$, are symmetric with respect to the permutation of $i$ and $j$, i.e., $\sum_{k} c_{ij}^{k} = \sum_{k} c_{ji}^{k}$. As a result

$$w_{\infty} = 0, \quad w_{n} = \sum_{k=1}^{n} \sum_{i,j=1}^{2} \epsilon_{ij}^{k} c_{ij}^{k}. \quad (13)$$

The sum rule, Eq. (13), together with Eq. (8) imply that the second order correction $\delta U_{12}^- \equiv u_2$ to the matrix element $U_{12}^-$ vanishes at high temperatures, when $\varepsilon_{k}^* = T$. More precisely, the usual Kondo logarithmic temperature dependence of $U_{12}^-$ persists only for $T < \varepsilon_{3} \equiv E_{3} - E_{1}$. Therefore, in the expression for $T_{K}$, Eq. (3), the bandwidth $D \sim \varepsilon_{F} \sim 5eV$ should be substituted by $\varepsilon_{3} \sim 3meV$:

$$T_{K} = \varepsilon_{3} (v_{x} v_{z})^{1/2} \left( \frac{v_{x}}{4v_{z}} \right)^{1/4} v_{x}. \quad (14)$$

It means that the Kondo temperature is about three orders of magnitude less than the “conventional” estimate!

To interpret this result note that when it tunnels, the heavy particle is under the barrier for a time $\sim h/\varepsilon_{3}$. At energies bigger than $\varepsilon_{3}$ we thus deal with a continuously moving particle rather than a pseudospin.

However, any truncation of the sum, Eq. (8), results in a strong overestimation of the Kondo temperature. Indeed, the truncated sum $w_{n}\ll\infty$, Eq. (13), is neither zero, nor exponentially small. Thus $u_{n} = w_{n} \ln(D/T) \gg u_{2}$ at least when $\varepsilon_{n} \ll T$. It is the substitution of $u_{\infty} \gtrsim u_{3}$, proposed in Ref. [3], that dramatically enhanced $T_{K}$.

The sum rule Eq. (13) hints that although contribution of each excited state $k$ to $u_{n}$ is quite large in absolute value (if $k$ is not too big), these contributions have different signs and cancel each other up to an exponentially small quantity $u_{\infty}$ when all of them are included.

To demonstrate that this is the case we repeated numerical calculations of Ref. [3], using the same model potential, Fig. 2, but took into account all of the excited states $\{k\}$ rather than only $k = 3$.

Following Ref. [3] we chose the barrier height to be $V = 9.86h_{2}/2M_{b}^{2}$, where $M$ is the particle mass and $b$ is the well width. We computed the eigenfunctions $\phi_{1}(x)$ and used Eqs. (3),(4),(6) and (8) to evaluate $\hat{u}_{n} \equiv u_{n}(k_{F}b)^{-2}$.

FIG. 2. Symmetric double well potential with the well width $b$, the barrier has a height $V$ and a width $2ab$.

Fig. 3 shows $n$-dependence of the ratios $y_{n} \equiv u_{n}/u_{2} = \hat{u}_{n}/\hat{u}_{2}$ (for $\varepsilon_{F} = 10^{3}\varepsilon_{3}$, $T = 0.00204\varepsilon_{3}$, and the relative width of the barrier $\alpha$ equal to 2.5). One can see that $y_{3} \gg 1$, i.e., $u_{3} \gg u_{2}$. As we expected, absolute values of $y_{3}, y_{5}, y_{6}$, are also large, but the signs alternate. In agreement with our analytical conclusions further increase of $n$ gradually reduces $|y_{n}|$, and $y_{n} \rightarrow y_{\infty} \sim 1$ when $n \rightarrow \infty$.

On the insets of Fig. 3 we present $\alpha$-dependencies of $y_{n}$ to make it evident that although $u_{n>2}$ is not exponentially small as $u_{2}$ is, it regains this smallness as $n \rightarrow \infty$. Indeed, $y_{34}$ is almost a constant in the interval $1.5<\alpha<3.0$ whereas $y_{6}$ increases with $\alpha$ by factor $\sim 5$ in the same interval, and $\ln(y_{6})$ is a linear function of $\alpha$. 

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that y curves coincide, i.e., \( \tilde{y} \) is presented on Fig. 4 in semilogarithmic scale. All four \( \alpha \) of the relative width of the barrier, \( y \) (insets). Upper inset: \( y_{34}(\alpha) \). The variation in the interval \( 2.5 < \alpha < 3.0 \) is less than 10\%. Lower inset: linear dependence of \( \ln(y_3) \) on \( \alpha \). Note that \( y_{3}(3)/y_{3}(2.5) \approx 5 \).

We also computed the temperature dependence of \( \tilde{u}_{30} \approx \tilde{u}_{\infty} \) as a function of the level number \( n \) and of the relative width of the barrier, \( \alpha \) (insets). The dependence is presented on Fig. 4 in semilogarithmic scale. All four curves coincide, i.e., \( \tilde{u}_{\infty} \) does not depend on \( \varepsilon_F \). Moreover, as it was expected, the logarithmic dependence, \( u_{\infty} \propto \ln(T) + \text{const} \), persists only as long as \( T < \varepsilon_3 \).

\[ \Delta_z \approx \left( \frac{4v_z}{v_x} \right)^\gamma \gg 1, \quad \gamma = \frac{1}{4v_x} - \frac{1}{2} \gg 1. \] (15)

The same conclusion can be reached for any double-well potential model. Therefore a movable defect weakly coupled with electrons is unable to demonstrate the two-channel Kondo non-Fermi liquid behavior.

Moreover, the estimate excludes the very possibility of the development of the strong coupling two-channel Kondo regime at arbitrary low temperatures: it implies that the splitting of the two lowest levels of a TLS, \( \Delta \), Eq. (2), always exceeds \( T_K \). Indeed, \( \Delta > \varepsilon_3 \gg \varepsilon_5 \gg \varepsilon_3 \approx \lambda (k_F a)^2 e^{-\gamma \varepsilon_3} \). Using the fact that the model is applicable only in the limit \( v_z \ll v_x \ll 1 \) we obtain

One can see that the numerical simulations unambiguously support the analytical conclusions. Taking into account the excited levels does not remove exponential smallness of the second order correction to the scattering amplitude. A similar problem with the similar solution - contribution of the continuous spectrum above the barrier to the \( \alpha \)-decay rate - is described in the book [16].

Returning to the Kondo temperature, Eq. (4), we find that \( T_K \ll 10^{-5} \) for the "typical parameters" Eq. (4) and an optimistic estimate \( \varepsilon_3 \approx 50 K \). Therefore the Kondo model based on movable structural defects is hardly able to explain the experiments, [11, 13, 14].

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[1] P. W. Anderson, B. I. Halperin and C. M. Varma, Philos. Mag. 25, 1 (1972); W. A. Phillips, J. Low. Temp. Phys. 7, 351 (1972).
[2] J. L. Black, in Glassy Metals I, edited by H. J. Günterodt and H. Beck (Springer, Berlin 1981), p. 245.
[3] R. W. Cochrane, R. Harris, J. O. Strom-Olson, and M. J. Zuckerman, Phys. Rev. Lett. 35, 677 (1975).
[4] J. Kondo, Physica (Utrecht) 57, 3366 (1997); P. Mohanty and R. A. Webb, Phys. Rev. Lett. 62, 211 (1980).
[5] A. Zawadowski, Phys. Rev. Lett. 50, 40 (1980).
[6] G. Zarán, A. Zawadowski, Phys. Rev. B 13, 599 (1998).
[7] D. L. Cox, A. Zawadowski, Adv. Phys. 47, 399 (1998).
[8] K. Vladár and A. Zawadowski, Phys. Rev. B 28, 1564, 1582 (1983); K. Vladár, G. Zimányi and A. Zawadowski, Phys. Rev. Lett. 56, 286 (1986).
[9] See, for a review, K. Vladár and A. Zawadowski, Phys. Rev. B 28, 1596 (1983).
[10] D. C. Ralph, A. W. W. Ludwig, J. von Delft, and R. A. Buhrman, Phys. Rev. Lett. 72, 1064 (1994).
[11] A. Zawadowski, Jan von Delft and D. C. Ralph, Phys. Rev. Lett. 83, 2632 (1999).
[12] P. Mohanty, E. M. Q. Jariwala, and R. A. Webb, Phys. Rev. Lett. 78, 3366 (1997); P. Mohanty and R. A. Webb, Phys. Rev. B 55, 145 (1997).
[13] M. Pierre, H. Pothier, D. Esteve, and N. O. Birge, Journ. of Low Temp. Phys., 118, 447 (2000).
[14] I. E. Smolyarenko, and N. S. Wingreen, Phys. Rev. B, 60, 9675, 1999; N. S. Wingreen, B. L. Altshuler, and Y. Meir, Phys. Rev. Lett., 75, 769 (1995).
[15] A. B. Migdal, "Qualitative methods in quantum theory", Reading, Mass., W.A. Benjamin (1977).
[16] Most features of the results obtained in Ref. [13] can be interpreted within a completely adiabatic renormaliza-
tion of mobile defects’ spectrum, see V. I. Kozub and A. M. Rudin, Phys. Rev. B 55, 259 (1997).

[18] The suppression of the tunneling splitting due to the orthogonality catastrophe $\Delta_z \rightarrow \tilde{\Delta}_z \equiv \Delta_z(\epsilon_3/T_K) - v_x^2$, slightly changes index in Eq. (15): $\gamma \rightarrow \tilde{\gamma} \equiv 1/(4v_x) - 1/2 - v_x$. One can see that $\tilde{\gamma} \approx \gamma \gg 1$, since $v_x \ll 1$. Therefore the inequality (15) remains valid even after taking into account the renormalization of $\Delta_z$. 