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

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A two-channel Kondo (2CK) non-Fermi liquid state in a metal resulting from the interaction between electrons and structural defects modeled by double-well potentials (DWP) is revisited. Account only of the two lowest states in DWP is known to lead to rather low Kondo temperature, $T_K$. We prove that the contribution of higher excited states *reduces* $T_K$, if *all* of the intermediate states are taken into account. Prefactor in $T_K$ is shown to be determined by the spacing between the second and the third levels $\epsilon_3$ in DWP rather than by the electron Fermi energy $\epsilon_F$. Since $\epsilon_3 \ll \epsilon_F$ there is no microscopic model of movable defects which may justify 2CK phenomenology.

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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 [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. [2] for a review.

It was proposed long ago [3] 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 (1D) Fermi gas of particles that are characterized by a *pseudospin* with components $\sigma = \pm$ as $\hat{\Psi}_{l=0} \equiv \hat{\Psi}_-$, $\hat{\Psi}_{l=1,m=0} \equiv \hat{\Psi}_+$, while the real electron spin index $s = \uparrow\downarrow$ is replaced with the channel index $\mu = 0, 1$. Furthermore, provided that the Fermi energy, $\epsilon_F$, exceeds all of the relevant energies, one can linearize the electron dispersion law near the Fermi level, $\varepsilon(p) \simeq v_F|p|$, where $v_F$ is the Fermi velocity. The divergences caused by the linearized spectrum should, thus, be cut off by the bandwidth $D \simeq \epsilon_F$. The resulting Hamiltonian of the system can be expressed as

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

Here the Pauli matrices, $\tau^{j}_{\sigma\sigma'}$, act in the space of the electron pseudospin, and $\hat{S}$ is the operator of the TLS pseudospin, $[S^i, S^j] = i\epsilon^{ijk} S_k$. 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 correspondingly 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 (2CK) Hamiltonian [4], 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. [5].

The 2CK 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, $\Delta = \sqrt{\Delta_x^2 + \Delta_z^2}$, do not exceed the Kondo temperature, $T_K$. It can be shown [6,7] that in the limit $v_z \ll v_x \ll 1$,

$$T_K = D(v_x v_z)^{1/2} (v_z/4v_x)^{1/4v_x}. \tag{2}$$

The non-Fermi liquid behavior of the TLS at the 2CK fixed point was used in Ref. [8] to interpret the zero bias anomaly in characteristics of point contacts [9] and more recently [10] to explain the temperature behavior of the dephasing rate observed in Refs. [11,12]. In general, TLS were assumed to play an important role in crystalline metals as well as in metallic glasses.

  

The assumptions of Ref. [10] were criticized in Ref. [13] on the grounds that the disorder induced splitting estimates were too high for the Kondo-like behavior to develop. Although several questions raised in Ref. [13] remain unanswered, we put this issue aside. Instead, we concentrate on a different objection — the smallness of $T_K$ in Eq. (2) for reasonable values of parameters. Here we prove that $T_K \ll \Delta_z$ for any set of the microscopic parameters, which allows the Kondo-like description, Eq. (1). Therefore, the 2CK fixed point by no means can be reached with the lowering of $T$ 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 $v_j$ and estimate them.

The coupling constant $v_x$ 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 $v_x$ at given Fermi wave number, $k_F$, and the size of TLS, $a$, as (see, e.g., [2,5]) $v_x \simeq \lambda k_F a$.

As to $v_z$, it characterizes the transition between the two states of the TLS assisted by an electron transition. The incoming electron renormalizes the barrier's height, $V$, and consequently the tunneling amplitude. However, the tunneling event still has to occur. Therefore, $v_z \simeq \lambda k_F^2 a^2 \exp(-\eta)$ [2,5], 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 $v_z$ is always much smaller than $v_x$, $v_z \simeq v_x (k_F a) \exp(-\eta) \ll v_x$, $\eta \simeq \hbar^{-1} a \sqrt{8MV}$. This is why $v_z$ was usually neglected in previous treatments of TLS. For "typical" values of the parameters

$$D \sim 5 \text{ eV}, \qquad v_x \simeq 0.2, \qquad v_z/v_x \simeq 10^{-3}, \tag{3}$$

the "conventional" estimate of the Kondo temperature is $T_K^c \simeq 10^{-2}$–$10^{-3}$ K [7]. 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 an attempt to resolve the problem of small $T_K$ the authors of Ref. [14] went beyond the two-level approximation and considered virtual tunneling through the third level of the "TLS." This contribution to $v_z$ apparently does not contain the tunneling exponent. According to Ref. [14], 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.

The Kondo temperature, $T_K$, can be extracted from second-order perturbation theory in the interaction of the tunneling particle with the electrons. We calculate the correction using the one-dimensional model [14].

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, $\sigma = \pm$:

$$U_{ij}^{\sigma_1\sigma_2} = 2\pi v_F \lambda I_{ij}^{\sigma_1\sigma_2}, \qquad I_{kl}^{\sigma\rho} \equiv \int dx\, \phi_k \phi_l \psi_\sigma \psi_\rho\,. \tag{4}$$

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. 1(a)]. (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. 1(b)].

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

$$\delta U_{ij}^{\sigma_1\sigma_2} \propto \lambda^2 v_F \sum_{j',\sigma} \int_{-D}^{D} \frac{d\xi\, (I_{ij'}^{\sigma_1\sigma} I_{jj'}^{\sigma_2\sigma} - I_{jj'}^{\sigma_1\sigma} I_{ij'}^{\sigma_2\sigma})}{(-\varepsilon_{j'} - \xi)(1 + e^{-\xi/T})}\,. \tag{5}$$

Here $I_{j;l}^{\sigma\rho}$ is determined by Eq. (4), $\xi$ denotes the energy of the intermediate electron or hole state counted from the Fermi level, and $\varepsilon_{j'} \equiv E_{j'} - E_1$ 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 $|\xi| < D \sim \epsilon_F$. As to the singularity at $\xi = -\varepsilon_k$, the integral in Eq. (5) should be understood as the principal value. The minus sign in front of the second (hole) term in the numerator is due to the anticommutation of fermionic operators.

Consider now matrix elements $U_{12}^{\sigma_1\sigma_2} = -U_{21}^{\sigma_1\sigma_2}$ that describe transitions of the heavy particle between its two lowest states. Using Eqs. (5) 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. (5). The result can be written as

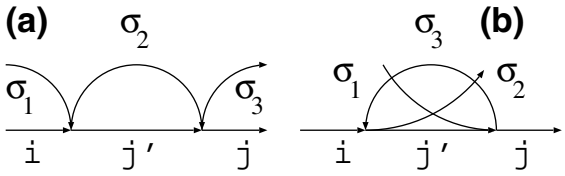


FIG. 1. Second-order diagrams for the scattering amplitude: (a) electron process and (b) hole process.

$$\frac{\delta U_{12}^{-+}}{U_{12}^{-+}} = \lambda u_\infty, \qquad u_n \equiv \frac{1}{I_{12}^{-+}} \sum_{k=1}^{n} \sum_{i,j=1}^{2} \epsilon^{ij} c_{ij}^k \ln\left(\frac{D}{\varepsilon_k^*}\right), \tag{6}$$

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

$$c_{ij}^k \equiv I_{ik}^{+-}(I_{jk}^{--} - I_{jk}^{++}), \qquad \varepsilon_k^* \equiv \max\{\varepsilon_k, T\}. \tag{7}$$

We start with the contribution of the first two levels ($k = 1, 2$) to the sum over $k$ in Eq. (6). Using Eqs. (5) and (7) one obtains, cf. with Ref. [14],

$$u_2 = \ln(D/T) \int dx\, [\phi_2^2 - \phi_1^2][\psi_-^2 - \psi_+^2]. \tag{8}$$

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), $\psi_-(x) \simeq \sqrt{2}[1 - (k_F x)^2/2]$, $\psi_+(x) \simeq \sqrt{2}\, k_F x$. We introduce the wave functions, $\phi_{l(r)}$, localized in the left (right) well, $\sqrt{2}\,\phi_{l,r} = \phi_1 \pm \phi_2$, recall that the functions $\phi_i$ are normalized, and rewrite Eq. (8) as

$$u_2 = 8 \ln(D/T) \int dx\, (k_F x)^2 \phi_l(x) \phi_r(x). \tag{9}$$

The wave functions $\phi_l(x)$ and $\phi_r(x)$ 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 $T_K$.

We show now that the account of the higher excited states in the double-well potential, i.e., terms with $k > 2$ in the sum Eq. (6), can only *reduce* the estimation of $T_K$.

Indeed, it follows from the definition of $I_{ij}^{\sigma\rho}$, Eq. (4), and completeness of the set of the functions, $\{\phi_k\}$, $\sum_k \phi_k(x)\phi_k(y) = \delta(x - y)$, that the sums, $\sum_k I_{ik}^{\sigma_1\sigma_2} I_{jk}^{\sigma_3\sigma_4}$ with any set $\sigma_n$, 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, $w_\infty = 0$, $w_n \equiv \sum_{k=1}^{n} \sum_{i,j=1}^{2} \epsilon^{ij} c_{ij}^k$. This sum rule allows one to rewrite Eq. (6) as

$$u_\infty = \frac{1}{I_{12}^{-+}} \sum_{k=1}^{\infty} w_k \ln\left(\frac{\varepsilon_{k+1}^*}{\varepsilon_k^*}\right). \tag{10}$$

This means that (i) high-energy cutoff $D$ drops out completely and (ii) the second-order correction (5) to the matrix element $U_{12}^{-+}$ *cannot contain logarithmic divergences at high temperatures,* $T \gtrsim \epsilon_3 \equiv E_3 - E_1$, $u_\infty \propto \ln(\epsilon_3/T)$, at smaller temperatures. On the other hand, the first iteration of the renormalization group (RG) equations must coincide with the logarithmically divergent term in the perturbation theory. This establishes the fact that the high-energy scale for the RG is $\epsilon_3$ rather than $D$. Precisely the same conclusion has actually been reached before in Ref. [15] in relation to a motion of a heavy particle in a metal. Therefore, in the expression for $T_K$, Eq. (2), the bandwidth $D \sim \epsilon_F \sim 5$ eV should be substituted by $\epsilon_3 \sim 3$ meV. As a result,

$$T_K = \epsilon_3 (v_x v_z)^{1/2} (v_z/4v_x)^{1/4v_x} \tag{11}$$

and *the Kondo temperature is about 3 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 $\sim\hbar/\epsilon_3$. At energies bigger than $\epsilon_3$ we thus deal with a continuously moving particle rather than a pseudospin. This physical conclusion is lost by any truncation of the sum, Eq. (6), which results in a strong overestimation of the Kondo temperature. Indeed, the truncated sum $w_{n<\infty}$ 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 $u_\infty$ by $u_3$, used in Ref. [14], that dramatically enhanced $T_K$.

The sum rule $w_\infty = 0$ hints that although the 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. [14], using the same model potential, Fig. 2, but took into account all of the excited states $\{k\}$ rather than only $k = 3$. Following Ref. [14] we chose the barrier height to be $V = 9.86\hbar^2/2Mb^2$, where $M$ is the particle mass and $b$ is the well width. We computed the eigenfunctions $\phi_i(x)$ and used Eqs. (6), (7), and (4) to evaluate $\tilde{u}_n \equiv u_n(k_F b)^{-2}$. Figure 3 shows $n$ dependence of the ratios $y_n \equiv u_n/u_2 = \tilde{u}_n/\tilde{u}_2$ (for $\epsilon_F = 10^3\epsilon_3$, $T = 0.002\,04\epsilon_3$, 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 $y_4, y_5, y_6$ are also large, but the signs alternate. In agreement with our analytical conclusions a further increase of $n$ gradually reduces $|y_n|$, and $y_n \to y_\infty \sim 1$ when $n \to \infty$.

In the insets of Fig. 3 we present $\alpha$ dependencies of $y_n$ to make it evident that although $u_{n>2}$ *is not as exponentially small* as $u_2$ is, it regains this smallness as $n \to \infty$. Indeed, $y_{34}$ is almost a constant in the interval $2.5 < \alpha < 3.0$, whereas $y_5$ increases with $\alpha$ by a factor of $\sim 5$ in the same interval, and $\ln(y_5)$ is a linear function of $\alpha$.

We also computed the temperature dependence of $\tilde{u}_{30} \simeq \tilde{u}_\infty$ for several Fermi energies. This dependence is presented in Fig. 4 in semilogarithmic scale. All four curves coincide, i.e., $\tilde{u}_\infty$ *does not depend on* $\epsilon_F$. Moreover, as was expected, the logarithmic dependence, $u_\infty \propto \ln(T) +$ const, persists only as long as $T < \epsilon_3$. One can see that

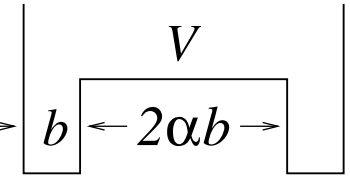


FIG. 2. Symmetric double-well potential with the well width $b$; the barrier has a height $V$ and a width $2ab$.

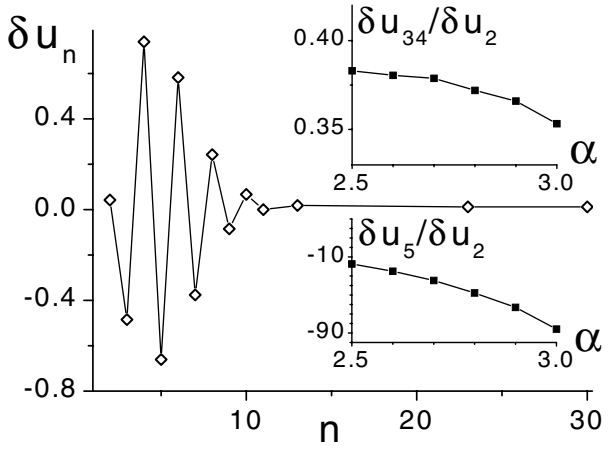


FIG. 3. $y_n \equiv u_n/u_2$ as a function of the level number $n$ and of the relative width of the barrier, $\alpha$ (insets). Upper inset: $y_{34}(\alpha)$. The variation in the interval $2.5 < \alpha < 3.0$ is less than 10%. Lower inset: linear dependence of $\ln(y_5)$ on $\alpha$. Note that $y_5(3)/y_5(2.5) \approx 5$.

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 a 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. (11), we find that $T_K \leq 10^{-5}$ for the "typical parameters" Eq. (3) and an optimistic estimate $\epsilon_3 \approx 50$ K. Therefore the Kondo model based on movable structural defects is hardly able to explain the experiments [8,11,12]. Finally, the estimate (11) excludes the very possibility of the development of the strong coupling 2CK regime at arbitrary low temperatures: the splitting of the two lowest levels of a TLS, $\Delta$, always exceeds $T_K$. Indeed, $\Delta \geq \Delta_z \simeq \epsilon_3 e^{-\eta} \gg v_z \epsilon_3 \simeq \lambda(k_F a)^2 e^{-\eta} \epsilon_3$. Because the model is applicable only if $v_z \ll v_x \ll 1$, we obtain

$$\Delta_z/T_K \gg (4v_x/v_z)^\gamma \gg 1\,, \qquad \gamma = 1/4v_x - 1/2 \gg 1\,. \tag{12}$$

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 2CK non-Fermi liquid behavior* [17].

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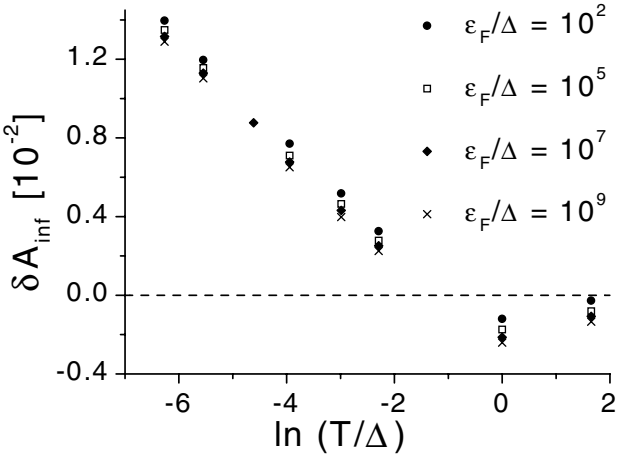


FIG. 4. The dependence of the quantity $\tilde{u}_{30} \equiv u_{30}(k_F b)^{-2}$ on $\ln(T/\epsilon_3)$ for different $\epsilon_F$ shown in the legend.

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