

Low Energy Properties of M -State Tunneling Systems in Metals: New Candidates for Non-Fermi-Liquid Systems

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We construct a generalized multiplicative renormalization group transformation to study the low energy dynamics of a heavy particle tunneling among M different positions and interacting with N_f independent conduction electron channels. Using a $1/N_f$ expansion we show that this M -level system scales towards a fixed point equivalent to the N_f channel $SU(M) \times SU(N_f)$ Coqblin-Schrieffer model. Solving numerically the scaling equations we find that a realistic M -level system scales close to this fixed point and its Kondo temperature is in the experimentally observable range 1–10 K. [S0031-9007(96)01492-5]

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One of the simplest examples of non-Fermi-liquid (NFL) systems is provided by the two-channel Kondo model [1–3], where the two conduction electron channels overcompensate the spin (or some quasi-spin) of an impurity and a new degenerate ground state appears with an intermediate coupling [1,2,4]. The FP corresponding to the ground state is characterized by nonzero residual entropy [3] and universal power law behavior in the impurity resistivity and the energy dependence of the scattering rate ($R_{\text{imp}} \sim T^{1/2}$, $1/\tau \sim \omega^{1/2}$) [2]. Several normal state properties of Ce or Y-based heavy fermion compounds like CeSn_3 and YbCuAl can also be explained surprisingly well in terms of the two-channel Kondo effect [5].

Other extensively studied possible realizations of the two-channel Kondo model are provided by fast two-level systems (TLS's) in metals [6,7]. These TLS's are formed by some heavy particles (HP's) tunneling between two neighboring sites and interacting strongly with the conduction electrons. Recent experimental [8] and theoretical [9,10] investigations confirm the conjecture that at low temperatures these TLS's can be properly described by an effective two-channel Kondo model, where the spatial motion of the HP is coupled to the angular momentum of the conduction electrons via an effective exchange coupling and the two degenerate channels correspond to the two real spin directions of the conduction electrons [8–10].

The TLS model sketched above is appropriate to describe tunneling centers in amorphous metals [11], however, it breaks down in systems like the narrow gap semiconductor $\text{Pb}_{1-x}\text{Ge}_x\text{Te}$ or insulating $\text{K}_{1-x}\text{Li}_x\text{Cl}$ alloys [12,13] where the tunneling centers are formed by some substitutional impurities, and the HP is tunneling between 3, 6, or 8 equivalent positions. Therefore the question arises in a natural way: What is the low temperature behavior of an M -level system (MLS) which strongly interacts with the conduction electrons?

To answer this question we consider a model previously introduced to describe the effect of the excited states in a

TLS [14]. In the following we assume that the temperature (or the relevant energy scale) is low enough and thus the motion of the HP is restricted to the lowest lying M states corresponding to the M spatial positions of the HP:

$$H_{\text{hp}} = \sum_{i,j=1}^M b_i^+ \Delta^{ij} b_j, \quad (1)$$

where b_i^+ creates a HP at site i and Δ^{ij} is the tunneling amplitude between positions i and j . We assume that no external stress is present and that the M positions are completely equivalent, thus $\Delta^{ii} = 0$.

The most general two-particle interaction generated by the screened Coulomb interaction (or a pseudopotential) between the HP and the conduction electrons takes the form

$$H_{\text{int}} = \sum_{\substack{i,j,n,m \\ \epsilon,\epsilon'}} b_i^+ V_{nm}^{ij} b_j a_{\epsilon n f}^+ a_{\epsilon' m f}, \quad (2)$$

where $a_{\epsilon n f}^+$ creates a conduction electron with energy ϵ , orbital quantum number n , and “flavor” index f ($f = 1, \dots, N_f$). The orbital quantum number n can be thought of as the angular momenta of the electrons while for a real MLS the quantum numbers $f = 1, 2$ correspond to the spin up and spin down conduction electrons and $N_f = 2$. For the sake of simplicity we also assume a constant density of states between the high and low energy cutoffs D and $-D$, ρ_0 , for all flavor numbers. Naturally, both the couplings V_{nm}^{ij} and the tunneling amplitudes Δ^{ij} are connected by the symmetry properties of the MLS which will be exploited later on.

Following similar lines as in Ref. [15] one can introduce the HP propagator $\mathcal{G}^{ij}(\omega)$ and the HP-conduction electron vertex function $\Gamma^{ij}(\omega)$ in the usual way. However, calculating these functions in a perturbative way it turns out that they do not satisfy the usual multiplicative renormalization group (RG) equations. Therefore we consider the following generalized RG transformation

($T = 0$):

$$\begin{aligned} \mathcal{G}(\omega, v', \Delta', D') &= A \mathcal{G}(\omega, v, \Delta, D) A^+, \\ \Gamma(\omega, v', \Delta', D') &= [A^+]^{-1} \Gamma(\omega, v, \Delta, D) A^{-1}, \end{aligned} \quad (3)$$

where the matrix notations $\varrho_0 V_{mn}^{ij} \rightarrow v$, $\Gamma_{mn}^{ij} \rightarrow \Gamma$, and $\Delta^{ij} \rightarrow \Delta$ have been introduced, D' stands for the scaled bandwidth, and A is an $M \times M$ matrix acting in the HP indices. Note that $A = A(v', \Delta', D'/D)$ is independent from the dynamical variable ω . While for finite D/D' the matrix A has a rather complicated structure for an infinitesimal change of D it can be chosen to be Hermitian and Eq. (3) can be cast in the form of a scaling equation for the dimensionless couplings v^{ij} .

In the following we assume that the relevant energy variable is ω , i.e., $\omega \gg |\Delta^{ij}|, T$. In this case the inverse

HP propagator and the vertex functions can be expressed in the next to leading logarithmic order [7] as

$$\begin{aligned} (\mathcal{G}^{-1})^{ij} &= \omega \delta^{ij} - \Delta^{ij} \\ &+ N_f \ln \frac{D}{\omega} (\delta^{ij} \omega \text{tr}\{v^{kl} v^{lk}\} - \text{tr}\{v^{ik} \Delta^{kl} v^{lj}\}) \\ \varrho_0 \Gamma^{ij} &= v^{ij} - \ln \frac{D}{\omega} ([v^{ik}, v^{kj}] - N_f \text{tr}\{v^{ik} v^{lj}\} v^{kl}), \end{aligned} \quad (4)$$

where $[,]$ denotes the commutator, the trace operator $\text{tr}\{\cdot\}$ is acting in the electronic indices, and a summation must be carried out over repeated indices. Plugging Eq. (4) into (3) one can easily generate the scaling equations in a self-consistent way:

$$\begin{aligned} \frac{d\Delta^{ij}}{dx} &= -\frac{1}{2} N_f [\text{tr}\{v^{ik} v^{kl}\} \Delta^{lj} + \Delta^{ik} \text{tr}\{v^{kl} v^{lj}\} - 2\text{tr}\{v^{ik} \Delta^{kl} v^{lj}\}] \\ \frac{dv^{ij}}{dx} &= -[v^{ik}, v^{kj}] + \frac{1}{2} N_f (2\text{tr}\{v^{ik} v^{lj}\} v^{kl} - \text{tr}\{v^{ik} v^{kl}\} v^{lj} - v^{ik} \text{tr}\{v^{kl} v^{lj}\}), \end{aligned} \quad (5)$$

where the scaling variable $x = \ln(D_0/D)$ has been introduced. Since the scaling equations are rather complicated apart from some special cases they can be solved only numerically. However, to exploit the symmetry properties of the MLS it is useful first to introduce some site representation in the orbital indices of the conduction electrons. This can be achieved most simply by taking some linear combinations of the most strongly scattered angular momentum channels and hybridizing them by using group theoretical methods. Working only with electron states directed to the impurity positions the v^{ij} 's become M^4 -dimensional tensors. However, the number of independent couplings is largely reduced by symmetry.

A typical scaling of the norm of the dimensionless couplings, $u = \sum \|v^{ij}\|$, is shown in Fig. 1 (dashed line). The initial couplings have been estimated by using similar methods as in Refs. [7,14]. Similarly to the multi-channel Kondo problem both the infinite and the weak coupling FP's are unstable and the system scales to an intermediate strong coupling FP [1,2,4]. The Kondo energy can be identified as the crossover energy from the weak to strong coupling regimes: $T_K = D_0 e^{-x_c}$, x_c being the crossover value of the scaling parameter. For realistic initial parameters we find that this Kondo temperature can easily be found in the experimentally observable region $T_K \sim 1-10$ K.

In order to determine the properties of the MLS in the regime $T, \omega \ll T_K$ one has to identify the FP the MLS scales to [16]. In the following we shall show that a MLS scales to a FP, which—up to some potential scattering part—has the same structure as the $SU(M) \times SU(N_f)$ Coqblin-Scrieffer model [17]. To prove this we first

remark that the operators $\delta^{ij} \sum_k v_{nm}^{kk}$ and $\delta_{mn} \sum_p v_{pp}^{ij}$ are invariant under scaling. Therefore v^{ij} can be written as $v_{mn}^{ij} = \tilde{v}_{mn}^{ij} + M_{mn}^{ij}$, where the matrix M is a constant of motion depending on the initial parameters and $\sum_i \tilde{v}_{nm}^{ii} = \sum_n \tilde{v}_{nm}^{ij} = 0$. Then one can easily show that the right-hand side of Eq. (5) disappears provided

$$\tilde{v}_0^{ij} = \frac{1}{N_f} \begin{pmatrix} O^{ij} & 0 \\ 0 & 0 \end{pmatrix}, \quad (6)$$

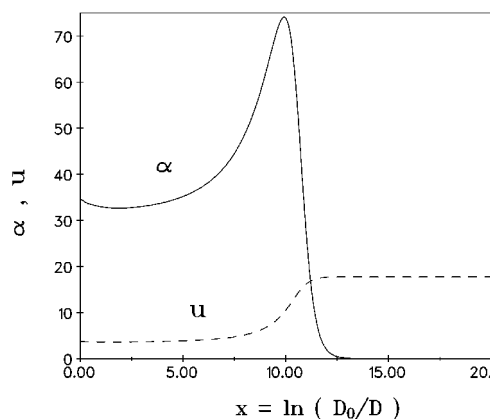


FIG. 1. Scaling of the norm of the dimensionless couplings, $u = \sum \|v^{ij}\|$ (dashed line), and of the algebra coefficient α (continuous line) for a six-state system with $N_f = 2$. The initial couplings have been chosen to be $v_{11}^{11} = 0.8$, $v_{22}^{11} = 0.2$, $v_{66}^{11} = 0.1$, $v_{12}^{11} = 0.05$, $v_{16}^{11} = 0.03$, $v_{21}^{12} = v_{12}^{12} = 0.0005$, $v_{11}^{12} = 0.005$, $v_{11}^{16} = 0.003$, $v_{61}^{16} = v_{16}^{16} = 0.0005$. The other nonzero couplings have been generated by symmetry transformations.

where the O^{ij} 's are unitary equivalent to the generators of the $SU(M)$ Lie algebra

$$[O^{ij}, O^{kl}] = \delta^{il} O^{kj} - \delta^{kj} O^{il}, \quad (7)$$

with $O_{nm}^{ij} \sim \delta_m^i \delta_n^j - \frac{1}{M} \delta^{ij} \delta_{nm}$. Similarly to the TLS problem beside the one in Eq. (6), Eq. (5) has an infinite number of FP's associated with different reducible and irreducible representations of the $SU(M)$ Lie algebra (7). Our numerical simulations show, however, that all the FP's which correspond to a representation different from the defining one (7) are unstable. In Fig. 1 we show the scaling of the "algebra coefficient" $\alpha = \sum_{i,j,k,l} \|N_f^2 [\tilde{v}^{ij} \tilde{v}^{kl}] - N_f \delta^{il} \tilde{v}^{kj} + N_f \delta^{kj} \tilde{v}^{il}\|$, which measures in a natural way how well the fixed point (6) is approached by the \tilde{v} 's. For $T < T_K$ (i.e., for $x > x_c$) the coefficient α scales to zero. Thus *below the Kondo temperature an MLS scales to the $SU(M) \times SU(N_f)$*

Coqblin-Schrieffer model, which is a non-Fermi-liquid model and has a different scaling behavior than the two-channel Kondo model [2,18]. (For a six-state system, e.g., we expect an $\omega^{1/4}$ behavior of the scattering rate.)

To show that FP (6) is stable and to analyze its operator content we write the deviations of the couplings from their FP value in a form

$$\delta v^{ij} = \begin{pmatrix} \rho^{ij} & t^{ij} \\ (t^{ji})^+ & \lambda^{ij} \end{pmatrix}, \quad (8)$$

and linearize the scaling equations with respect to δv^{ij} . The couplings ρ^{ij} , t^{ij} , and μ^{ij} are $M \times M$, $M \times \infty$, and $\infty \times \infty$ matrices, respectively. Like the TLS case the linearized equations for ρ^{ij} , t^{ij} , and μ^{ij} decouple completely,

$$\frac{d\mu^{il}}{dx} = \frac{1}{N_f} (\delta^{ij} \mu^{kk} - M \mu^{il}), \quad (9)$$

$$\begin{aligned} \frac{d\rho^{il}}{dx} = & -\frac{1}{N_f} ([O^{ik}, \rho^{kl}] + [\rho^{ik}, O^{kl}]) + \frac{1}{2N_f} \{2\delta^{il} \rho^{kk} + 2O^{jk} \text{tr}\{\rho^{ij} O^{kl} + O^{ij} \rho^{kl}\} \\ & - 2n \rho^{il} - O^{ij} \text{tr}\{\rho^{jk} O^{kl} + O^{jk} \rho^{kl}\} - \text{tr}\{\rho^{ij} O^{jk} + O^{ij} \rho^{jk}\} O^{kl}\}, \end{aligned} \quad (10)$$

$$\frac{dt^{il}}{dx} = -\frac{1}{N_f} (O^{ik} t^{kl} - O^{kl} t^{ik}) + \frac{1}{N_f} (\delta^{il} t^{kk} - M t^{il}), \quad (11)$$

and they can be solved exactly due to the simple structure of the O^{ij} 's. These linearized equations have an infinite number of zero modes; a finite number of them correspond to potential scattering while the others can be identified with the generators of the unitary transformations connecting the different possible M -dimensional subspaces where the $SU(M)$ Lie algebra is realized. These 0-modes can be shown, of course, to leave the Lie algebra (7) unaffected. All the other modes can be shown to be irrelevant, thus the FP (6) is stable.

The low energy properties of the MLS are determined by the operator content of the FP which is much richer and quite different from that of the simple Coqblin-Schrieffer model. A thorough analysis of Eq. (11) shows that for $M \geq 3$ the leading irrelevant operators can be written as

$$O_l \sim \begin{pmatrix} 0 & C^{ij} \\ (C^{ji})^+ & 0 \end{pmatrix}, \quad (12)$$

where the C^{ij} 's satisfy $\sum_l (C_{mn}^{kl} - C_{kn}^{ml}) = 0$. These operators scale like $\sim T^{\lambda_l}$ with $\lambda_l = (M-1)/N_f$, and they describe scattering between channels which are not taken into account in the usual Coqblin-Schrieffer model. While they dominate the thermodynamical quantities like the specific heat, e.g., which scales as $c_{\text{imp}} \sim T^{2\lambda_l}$ they do not contribute to the resistivity, which scales like $\sim T^{\lambda_{sl}}$ with $\lambda_{sl} = M/N_f$, and is determined by sublead-

ing operators of the form

$$O_{sl} \sim \begin{pmatrix} Q^{ij} & 0 \\ 0 & S^{ij} \end{pmatrix}, \quad (13)$$

where the matrices Q^{ij} and S^{ij} satisfy $\sum Q^{ii} = \sum S^{ii} = 0$ and $Q_{mn}^{ij} = Q_{nm}^{ij}$. Note that the operators (12) do not exist in the TLS case ($M=2$), and therefore the low energy properties of a TLS can be completely described by the two-channel Kondo model [10].

At this point we have to remark that since the FP couplings \tilde{v}^{ij} scale like $1/N_f$ the obtained scaling exponents can be considered as the first order estimates in a $1/N_f$ expansion, and they become exact in the $N_f \rightarrow \infty$ limit [10,19] ($\lambda_{sl} = M/N_f$ is, e.g., the $1/N_f$ -expanded version of the exact exponent $\tilde{\lambda}_{sl} = M/(N_f + M)$ for $N_f > M$ [2,18]). However, the $1/N_f$ expansion breaks down for $N_f < M$, and while for a physical MLS with $N_f = 2$ we expect similarly to other models [7,10] that the *fixed point structure* remains the same; it remains an open question whether the new leading irrelevant operators (12) survive in that physical limit or not.

In order to decide whether or not the non-Fermi-liquid properties can be recovered in reality, it is important to study the scaling of the splitting Δ^{ij} . As soon as the temperature (frequency) becomes smaller than the renormalized splitting $|\Delta^{ij}(T, \omega)|$ the dynamics of the MLS is frozen out and the Kondo effect described above is stopped. Therefore in order to observe a non-Fermi-liquid behavior characteristic to the FP (6) we need $|\Delta^{ij}(T_K)| \ll T_K$. The scaling of the splitting parameter Δ^{12} is shown in Fig. 2 (for the definition of Δ^{12} , see

the inset in Fig. 2). As one can see, for realistic model parameters $\Delta^{12}(T_K)/\Delta^{12}(D_0)$ is as small as $\sim 10^{-3}$, and therefore, even for very large splittings $\Delta^{12} \sim 100$ K the splitting is strongly reduced and since $\Delta^{12}(T_K) \ll T_K$ the MLS can get easily in the vicinity of the two-channel Coqblin-Schrieffer FP.

As recently pointed out by Moustakas and Fisher for TLS's [20] multielectron scattering becomes also relevant in the neighborhood of the two-channel Kondo fixed point. This process is also relevant in the present model in the vicinity of the NFL fixed point, however, similarly to the TLS case [21] it has a small initial amplitude, and being irrelevant in the weak coupling region this amplitude is even more significantly reduced during the first part of the scaling, $T_K < D < D_0$. Therefore, in the neighborhood of the FP (6) it is always the splitting Δ^{ij} discussed above which provides the dominant mechanism to drive the system away the NFL FP and the multielectron processes play a less important role.

Concerning the experimental realizations there exist already some experiments on noncommutative eight-state systems in $\text{Pb}_{1-x}\text{Ge}_x\text{Te}$ alloys where the tunneling centers are formed by the relatively small Ge^{++} ions [12]. While in this material a Kondo crossover has indeed been observed no non-Fermi-liquid behavior has been detected. However, in the experiments the inter-impurity interaction was quite strong which leads to the nonvanishing of the diagonal part Δ^{ii} of the tunneling matrix. Since, similarly to TLS's, the differences $\Delta^{ii} - \Delta^{jj}$ are renormalized much less than the off-diagonal matrix elements [7], they can lead to the freezing out of some impurity states corresponding to transitions from the $\text{SU}(M)$ to $\text{SU}(M')$ models with $M' < M$, finally, most probably, reaching the trivial $M' = 1$ model. Furthermore, in this material there is a strong spin-orbit scattering, which leads to a strong cross scattering between the spin up and spin down electron channels and drives the system to the $N_f = 1$ Fermi-liquid FP instead of the $N_f = 2$ non-Fermi-liquid model. Thus for this material even if the inter-impurity interactions were small we would expect a Fermi liquid behavior. Therefore it would be very interesting from the

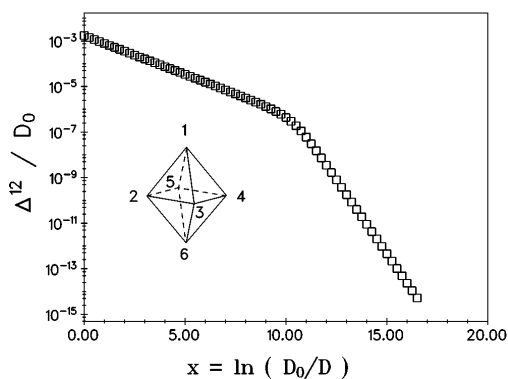


FIG. 2. Scaling of the dimensionless hopping amplitude Δ^{12}/D_0 for the same six-state system as in Fig. 1. Inset: Numbering of the sites of the six-state system.

experimental side to find some similar alloys with *small spin-orbit interaction*, where the spin symmetry would guarantee the non-Fermi-liquid properties. To observe the non-Fermi liquid FP one could apply a pressure on the sample, which is an appropriate tool for tuning T_K into the region 1–10 K [12].

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