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Absence of two energy scales in the two-impurity Kondo model

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It is believed that the successive antiferromagnetic scattering of the conduction electrons on two magnetic impurities in a metal, induces a magnetic interaction between the impurities which sets an energy scale for the system, in addition to the Kondo temperature. However, it is shown here that this contradicts a scaling law for the two-impurity Anderson model in the magnetic limit which becomes exact for a large bandwidth. [S0163-1829(98)50212-3]

In heavy fermion materials localized, strongly correlated f electrons interact with delocalized, weakly correlated conduction electrons. Experiments show that above a temperature T^* the magnetic moments of the f electrons behave asymptotically as free. Well below T^* they can either be phenomenologically described as a Fermi liquid, or magnetic correlations between the local f moments become dominant.[1]

When searching for a microscopic mechanism, one is guided by the behavior of dilute magnetic alloys which are well described by the single-impurity Anderson Hamiltonian.[2] At low temperatures the magnetic moment of the impurity is screened by particle-hole excitations of the conduction band. The system behaves universally, that is, all observables scale with one energy $k_B T_K$ where T_K is called the Kondo temperature. On the other hand, the heavy fermion materials have, in orders of magnitude, one magnetic ''impurity'' atom per unit cell. The hypothesis for such systems is that it can be described by the Anderson-lattice Hamiltonian.

It is far from obvious why the single-impurity Kondo effect should survive in the lattice model. It is believed that magnetic interactions between the local f moments compete with the Kondo effect. This magnetic interaction between the local f moments is supposed to be induced by successive scattering of the conduction electrons on the two impurities, and called Ruderman-Kittel or RKKY interaction.[3–5] Doniach[4] estimated how much energy the system gains if it orders antiferromagnetically. By second-order perturbation theory in the exchange coupling J between the conduction and the f electrons this RKKY energy was found to be of the order

$$I \propto \rho^2 J^2 D,$$

where ρ is the density of states at the Fermi energy of the conduction band of width D. Doniach compared it with the exponentially small energy gain

$$k_B T_K \propto D \exp[-1/(\rho J)],$$

if the magnetic atoms are considered to be independent magnetic impurities. Depending on the size of J, it could then be estimated whether the material is in a magnetic or nonmagnetic phase, at low temperatures. This simple picture deals essentially with a two-impurity Hamiltonian, the standard version of which is the two-impurity Anderson or Kondo model. It has had great impact on the experimentalist's point of view. In fact, standard reviews quote the Doniach picture to explain, at least qualitatively, the respective experimental observations.[1,6]

In this article it will be shown that this simple picture cannot be valid. To this end let us discuss firstly the various approaches to the two-impurity problem.

For the two-impurity Kondo model, summing of leading-order divergent diagrams[7] in the spirit of Abrikosov[8] showed that at decreasing temperature, the RKKY interaction as well as the Kondo interaction are renormalized, and eventually diverge at low temperatures. Hence the picture drawn by Doniach would be invalid.

This can be contrasted with results from poor man's scaling:[5,9] Depending on the distance between the impurities, the RKKY interaction I may either be ferro- or antiferromagnetic. If I is ferromagnetic and larger than $k_B T_K$, it is predicted that the magnetic moments of the two impurities first form an effective spin one and are then quenched in a two-stage process, as temperature decreases. On the other hand, a large antiferromagnetic RKKY interaction suppresses the Kondo effect and the two-impurity spins form a singlet for $k_B T < I$. It is then argued that I sets an energy scale for the system at which the RKKY interaction could be observed.

This analysis was supported by a more recent calculation with the help of a variant of the numerical renormalization group by Silva *et al.*[10,11] (in which the Nth hopping matrix element of the half-infinite chain to which the two impurities couple is vanishing as Λ^{-N} with $\Lambda = 10$, and subsequently the results of different bandwidths D/Λ^{ϵ}, $\epsilon = 0 \ldots 1$ are averaged over). In fact, those results imply that the Doniach picture is *valid*.

However, those results contradict others[12] using the conventional renormalization group scheme ($\Lambda = 3$) where only one low-energy scale was seen. What is more, the approaches of Refs. 5, 9, and 10 are inconsistent. To clarify the point, only the case of an antiferromagnetic RKKY interaction is discussed. Silva *et al.* interpreted their data with the help of poor man's scaling. They saw that the magnetic moment of the impurities is quenched as temperature decreases below I/k_B, at which temperature I and J themselves are not much renormalized. They claimed that therefore the two impurities would form a singlet for $k_B T < I$, consequently the renormalization of J would stop, and the low-temperature behavior could be determined from perturbation theory, the lowest nonvanishing order of which is $\propto J^2/I$. A simple estimation shows however that this perturbative expansion is not allowed: Because $\rho \propto 1/D$, the RKKY interaction I is

always a factor J/D *smaller* than the Kondo interaction J. This can be read off their numerical results as well.[10]

Incidentally, if the arguments given by Silva *et al.* were correct they could be repeated for the antiferromagnetic single-impurity Kondo model: At a temperature of the order of the coupling constant J the impurity spin and an electron of the conduction band would form a singlet, the renormalization would stop, and one would be left with a ''Kondo effect'' at an energy scale of the order of J, which is certainly not true.

To summarize, the Doniach picture and its subsequent refinements as described above imply that the renormalization of J stops as temperature becomes lower than the RKKY coupling. This RKKY interaction then sets an energy scale for the system's response, at least for small coupling $J \ll D$. Therefore it would be helpful if the exact energy scales of a metal with two magnetic impurities could be calculated in the universal limit of large D. The method which is usually employed for that purpose is the diagrammatic renormalization group. The major obstacle is the solution of the Dyson equation connecting the dressed propagators and their self-energies which can be done only perturbatively. However, the low-energy behavior is beyond perturbation theory. An explicit solution of the Dyson equation can be avoided[13] by means of the variational principle of Luttinger and Ward[14–16] with the help of which the energy scales will follow.

The two-impurity Anderson model serves here as the standard model for two magnetic impurities in a metal. Mean-field approaches for this model have the drawback that the RKKY interaction appears only as a higher-order correction,[17] and therefore a magnetic interaction between the impurities had to be added by hand, giving a model with an adjustable strength of the magnetic exchange between the impurities.

Here, however, a direct exchange interaction between the impurities will *not* be taken into account, because the two impurities model two localized f orbitals on different lattice sites, with virtually no overlap, and it is the purpose of this article to investigate the role of their *induced* magnetic interaction, that is, the RKKY interaction.

The two impurities are assumed to sit at $(0,0,\pm R/2)$ symmetrically to the origin of the coordinate system, along the z axis. The Hamiltonian H is then invariant under the parity transformation. Hence the creation operator for a conduction electron of momentum p and spin m and for an impurity electron can be expressed in terms of their even $(\sigma=1)$ and odd $(\sigma=-1)$ combinations,[18,19]

$$c^{+}_{\vec{p},m,\sigma}=\frac{1}{\sqrt{2}}(c^{+}_{\vec{p},m}+\sigma c^{+}_{-\vec{p},m}),$$

$$f^{+}_{\sigma m}|\mathrm{vac}\rangle=\frac{1}{\sqrt{2}}(f^{+}_{1m}+\sigma f^{+}_{2m})|\mathrm{vac}\rangle,$$

$$d^{+}_{\sigma mn}|\mathrm{vac}\rangle=-\sigma d^{+}_{\sigma nm}|\mathrm{vac}\rangle=\frac{(\sigma f^{+}_{1m}f^{+}_{2n}-f^{+}_{1n}f^{+}_{2m})}{\sqrt{2(1+\delta_{mn})}}|\mathrm{vac}\rangle. \quad (1)$$

Here $c^{+}_{\vec{p}m}$ creates a conduction electron with internal quantum number $m=1\ldots N$, momentum $\vec{p}$, and energy $\epsilon(\vec{p})$. If $|\mathrm{vac}\rangle$ is the vacuum, then $b^{+}|\mathrm{vac}\rangle$, $f^{+}_{im}|\mathrm{vac}\rangle$, and $d^{+}_{mn}|\mathrm{vac}\rangle$ denote the unoccupied, singly occupied, and doubly occupied impurity configurations, with $i=1,2$ labeling the impurities. The energy difference between the singly occupied and unoccupied as well as between the doubly and singly occupied impurity configuration is ϵ_f. f^{+}_{im} is a fermionic operator, and b^{+} and d^{+}_{mn} are bosonic. Double occupancy at each impurity site is suppressed by requiring $b^{+}b+\Sigma_{\sigma m}f^{+}_{\sigma m}f_{\sigma m}+\Sigma_{\sigma,m\geqslant n}d^{+}_{\sigma mn}d_{\sigma mn}\equiv 1$. The unoccupied configuration $b^{+}|\mathrm{vac}\rangle$ has even parity. The effective Hamiltonian then reads,[19]

$$H=H_c+H_f+H_1,$$

$$H_c=\sum_{\epsilon\sigma}\epsilon c^{+}_{\epsilon m\sigma}c_{\epsilon m\sigma},$$

$$H_f=\epsilon_f\sum_{m\sigma}f^{+}_{\sigma m}f_{\sigma m}+2\epsilon_f\sum_{m\geqslant n,\sigma}d^{+}_{\sigma mn}d_{\sigma mn},$$

$$H_1=\frac{1}{\sqrt{N}}\sum_{\epsilon,m,\sigma}V_\sigma(\epsilon)(f^{+}_{\sigma m}bc_{\sigma\epsilon m}+\mathrm{H.c.})$$

$$+\frac{1}{\sqrt{2N}}\sum_{\epsilon,m\neq n,\sigma,\tau}\tau V_\tau(\epsilon)(d^{+}_{\sigma\tau,mn}f_{\sigma n}c_{\tau\epsilon m}+\mathrm{H.c.})$$

$$+\frac{1}{\sqrt{N}}\sum_{\epsilon,m,\sigma}\sigma V_\sigma(\epsilon)(d^{+}_{-1,mm}f_{-\sigma m}c_{\sigma,\epsilon m}+\mathrm{H.c.}). \quad (2)$$

The impurity hybridization with the conduction band is proportional to V. The Boltzmann constant is set to unity so that temperature is measured in units of energy. The dispersion can be assumed as isotropic. The density of states ρ is assumed to be constant, and the such linearized dispersion is cut off at $\pm D$. The effective hybridization matrix element can then be expressed in terms of the conduction band density of states as[19]

$$V_\sigma(\epsilon)=V\sqrt{\rho}\Theta\left(1-\frac{\epsilon^2}{D^2}\right)\sqrt{1+\sigma\frac{\sin[k_FR(1+\epsilon/2D)]}{k_FR(1+\epsilon/2D)}}, \quad (3)$$

with k_F the Fermi wave number and Θ the step function. Thus the system has been reduced to an effective one-impurity Hamiltonian, the additional parity quantum number keeping track of the original two impurities.

The one-particle impurity propagators R_f for the unoccupied $(f=0)$, singly occupied $(f=\sigma m)$, and doubly occupied $(f=\sigma mn)$ impurity configurations, determine the impurity part Z_f of the partition function via a line integral, the path of integration encircling all poles of the integrand,

$$Z_f:=\frac{\mathrm{Tr}_f\ \mathrm{Tr}_c e^{-\beta H}}{\mathrm{Tr}_c e^{-\beta H_c}}=\mathrm{Tr}_f\oint\frac{dz}{2\pi i}e^{-\beta z}R_f(z), \quad (4)$$

where Tr_f denotes the trace over the impurity configurations. The propagators R_f can be calculated by the standard dia-

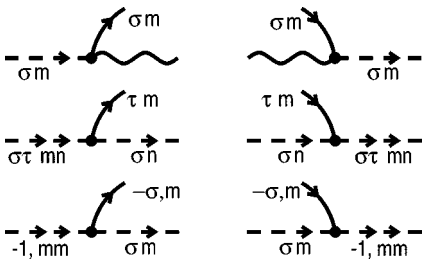

FIG. 1. Vertices for the two-impurity Anderson model. A dashed, singly or doubly arrowed line represents the naked propagator of the singly or doubly occupied impurity configuration. A single σ or τ labels the parity ± 1, and $\sigma\tau$ their product. m or n labels the magnetic quantum number, and mn a pair of magnetic quantum numbers for the double occupied configuration. A wavy respective solid line represents the naked propagator of the unoccupied impurity configuration or the conduction electron. The product of parities of incoming particles equals that of the outgoing ones.

grammatic technique[19] which is reviewed in Ref. 20. The vertices and naked propagators are shown in Fig. 1.

Within the variational principle,[15] a functional Υ of the propagators R_f is defined in terms of skeleton diagrams. For the impurity part of the partition function, Υ is given by

$$\Upsilon=\beta\ \mathrm{Tr}_f\ \oint\ \frac{dz}{2\pi i}e^{-\beta z}\Bigg\{\sum_n\ \left(1-\frac{1}{n}\right)\Sigma_f^{(n)}(R_f(z))R_f(z) + \ln\Bigg[z-H_f-\sum_n\ \Sigma_f^{(n)}(R_f(z))\Bigg]\Bigg\}. \tag{5}$$

Here $\Sigma_f^{(n)}$ denotes the nth order self-energy of R_f, expressed in terms of skeleton diagrams. At the saddle point with respect to variations of R_f, the functional Υ equals Z_f and the Dyson equation holds as a self-consistency equation.[15] So Υ depends on parameters such as ϵ_f explicitly only via H_f, and not implicitly via the propagators.[15] In addition, Υ depends explicitly on V only via the prefactor V^{2n} of the $2n$th order self-energy $\Sigma_f^{(2n)}$. To determine the T dependence, the internal integration variables z and ϵ, as in Eqs. (5) and (7) are replaced by Tz, $T\epsilon$, and D/T, respectively. The variational principle remains unaffected. Υ depends now explicitly on T via the prefactor T^n of a skeleton diagram of $2n$th order, the term Tz in the logarithm, and D/T because of Eq. (3). Similar to Ref. 13, it follows for the impurity part F_f of the free energy

$$F_f=\left(T\frac{\partial}{\partial T}+\rho V^2\frac{\partial}{\partial\rho V^2}+\epsilon_f\frac{\partial}{\partial\epsilon_f}+D\frac{\partial}{\partial D}\right)F_f. \tag{6}$$

Approximations fulfilling the variational principle can be generated by using a subclass, the so-called families of skeleton diagrams.[21] If, for instance, only the family of second-order skeleton diagrams is kept in Υ, the self-energies are (f denotes the Fermi function),

$$\Sigma^{(2)}_{\sigma\tau,mn}(z)=\frac{1}{2N}\sum_{\sigma\tau=\mathrm{const}}\ \int d\epsilon f(\epsilon)V_\tau^2(-\epsilon)[R_{\sigma n}(z+\epsilon)+R_{\sigma m}(z+\epsilon)],$$

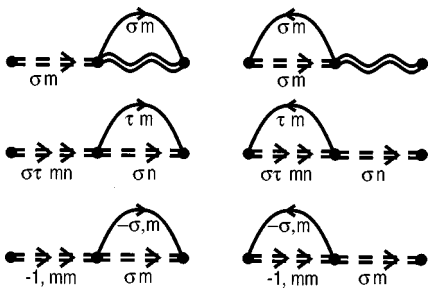

FIG. 2. Skeleton diagrams of second order for the two-impurity Anderson model

$$\Sigma^{(2)}_{\sigma m}(z)=\frac{1}{N}\int d\epsilon f(\epsilon)\Bigg[\frac{1}{2}\sum_{\tau n\neq m}V_\tau^2(\epsilon)R_{\sigma\tau,mn}(z+\epsilon) + V_\sigma^2(-\epsilon)R_0(z+\epsilon)+V_{-\sigma}^2(\epsilon)R_{-1,mm}(z+\epsilon)\Bigg],$$

$$\Sigma_0^{(2)}(z)=\frac{1}{N}\sum_{\sigma,m}\int d\epsilon f(\epsilon)V_\sigma^2(\epsilon)R_{\sigma m}(z+\epsilon). \tag{7}$$

Universal behavior of the system manifests itself when D becomes larger than all other energy scales of the system. Υ depends explicitly on D only via V_σ^2, as in Eq. (3),

$$D\partial_D\Upsilon=-\mathrm{Tr}_f\ \oint\ \frac{\beta dz}{2\pi i}e^{-\beta z}D\partial_D\sum_n\ \frac{1}{n}\Sigma_f^{(n)}(z)R_f(z). \tag{8}$$

The skeleton diagrams for $\Sigma_f^{(2)}R_f$ are shown in Fig. 2.

The effective density of states of Eq. (3) scales with D as a function of ϵ and is finite at the Fermi energy $\epsilon=0$. Hence,[13] as in the case for a density of states with a sharp cutoff at $\pm D$, differentiating a skeleton diagram for $\Sigma_f^{(n)}R_f$ with respect to D amounts to removing one curved conduction electron line and replacing the internal propagator by its value at the cutoff $\propto 1/D$. Therefore a skeleton diagram of second order contributes $\propto D/D$ to the logarithmic derivative.

A skeleton diagram of higher than second order contains vertex corrections; hence there lie under each conduction electron line at least two impurity propagators, because otherwise this diagram would have a self-energy insertion and not be a skeleton. Its contribution to the logarithmic derivative is therefore $\propto D/D^2$ and can be neglected for large D.[13]

Therefore, in Eq. (8) only the skeleton diagrams for $\Sigma_f^{(2)}R_f$ are necessary to obtain the exact energy scales of the system in the universal limit of large D. A spectral decomposition of the impurity propagators yields,

$$D\frac{\partial}{\partial D}F_f=-\int\ \frac{e^{-\beta\omega}d\omega}{NZ_f}\Bigg\{\sum_{\sigma,m}V_\sigma^2(0)[\rho_{\sigma m}(\omega)+\rho_0(\omega)] + \frac{1}{2}\sum_{\sigma\tau,m\neq n}V_\tau^2(0)[\rho_{\sigma\tau mn}(\omega)+\rho_{\sigma n}(\omega)] + \sum_{\sigma,m}\ [V_\sigma^2(0)\rho_{-1,mm}(\omega)+V_{-\sigma}^2(0)\rho_{\sigma m}(\omega)]\Bigg\}.$$

Together with the identities

$$Z_f = \int e^{-\beta\omega} d\omega \left[\rho_0(\omega) + \sum_{\sigma,m} \rho_{\sigma m}(\omega) + \sum_{\sigma,m\geqslant n} \rho_{\sigma mn}(\omega) \right],$$

$$Z_f \frac{\partial}{\partial \epsilon_f} F_f = \int e^{-\beta\omega} d\omega \left[\sum_{\sigma,m} \rho_{\sigma m}(\omega) + 2 \sum_{\sigma,m\geqslant n} \rho_{\sigma mn}(\omega) \right],$$

the following scaling equation is obtained:

$$D \frac{\partial}{\partial D} F_f = \rho V^2 (1 - 1/N) \frac{\partial}{\partial \epsilon_f} F_f - 2\rho V^2. \tag{9}$$

Equations (6) and (9) imply the scaling law

$$F_f - E_0 = T g(T, V, \epsilon_f, D, \rho) = T g\left(\frac{T}{\Gamma}, \frac{T}{T_K} \right) \tag{10}$$

in the magnetic limit $-\epsilon_f \gg \rho V^2$, with $\Gamma = \pi \rho V^2 / N$. In this limit, the Anderson model is equivalent to the two-impurity Kondo model[22] at low temperatures $T \ll \rho V^2$, with $T_K = D \sqrt[N]{\rho V^2 / D}\, \exp[\epsilon_f / \rho V^2]$. By the same means[13] it can be shown that in this limit all observables scale as in Eq. (10).

Hence the two-impurity Kondo model has in the limit of large D only *one* low-energy scale, which is proportional to the single-impurity Kondo temperature. Observe, however, that the proportionality factor cannot be fixed within this approach and will of course depend on $k_F R$.

If the RKKY interaction would set additional energy scales as discussed in the introduction, then the scaling law would have the form,

$$F_f - E_0 = T g\left(\frac{T}{T_K}, \frac{T}{I}, \frac{T}{T_{KA}}, \frac{T}{T_+} \right), \tag{11}$$

where T_{KA} and T_+ are the temperatures of the two-stage Kondo effect for the ferromagnetic RKKY interaction.[5,9] This, however, contradicts the scaling law (10) above.

To conclude, if the high-energy cutoff of the metal is so large that terms of the order T/D or J/D can be neglected, there is for two magnetic impurities in a metal only one low-energy scale. The induced indirect exchange interaction between the local f moments which is mediated by successive scattering of conduction electrons, will be strongly renormalized at low temperatures. However, the scaling equations alone do not predict the nature of the ground state for two magnetic impurities in a metal. In view of Eq. (10) it seems doubtful whether a competition between the formation of magnetic order and a Fermi liquid of heavy quasiparticles can be understood without adding explicitly a magnetic interaction between the magnetic f moments.

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