Relation between the Anderson and Kondo Hamiltonians

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A canonical transformation is used to relate the Anderson model of a localized magnetic moment in a dilute alloy to that of Kondo. In the limit of small *s-d* mixing, which is the most favorable case for the occurrence of a moment, the two models are shown to be equivalent. The Anderson model thus has low-temperature anomalies similar to those previously discussed for the Kondo model.

WE have investigated the Anderson model of a localized magnetic moment in a dilute alloy[1] for the limiting case which is most favorable for a localized moment to occur, namely small *s-d* mixing. We find that Anderson's Hamiltonian can be transformed to a form similar to that of the *s-d* exchange model used by Kondo,[2] with an energy-dependent antiferromagnetic exchange interaction $J_{kk'}$. Since the Kondo effect apparently leads, at sufficiently low temperature, to a condensation in which a localized conduction-electron spin polarization compensates the impurity moment,[3] we conclude that the Anderson model does not lead to a localized magnetic moment at zero temperature. For temperatures high compared to the condensation temperature T_c the impurity moment presumably breaks free from the conduction-electron polarization cloud and a localized moment appears. Thus, the existence of a localized moment in the Anderson model for a given temperature range depends critically on the strength of the effective exchange interaction $J_{kk'}$.

The Anderson Hamiltonian for a single localized orbital "d" is

$$H=\sum_{ks}\epsilon_k n_{ks}+\sum_s \epsilon_d n_{ds}+Un_{d\uparrow}n_{d\downarrow}+\sum_{ks}\{V_{kd}c_{ks}^{\dagger}c_{ds}+V_{kd}^{*}c_{ds}^{\dagger}c_{ks}\}, \quad (1)$$

where ϵ_k and ϵ_d are the one-electron energies of the conduction and localized orbitals, measured relative to the Fermi energy. The d and k states are mixed by the potential V; U is the Coulomb repulsion between opposite-spin electrons located on the d orbital. The model can be characterized by two dimensionless ratios

$$r_{\pm}\equiv\Gamma_{\pm}/|\epsilon_{\pm}|, \quad (2a)$$

where

$$\epsilon_{\alpha}=\epsilon_d+U, \quad \alpha=+; \qquad =\epsilon_d, \quad \alpha=-; \quad (2b)$$

and

$$\Gamma_{\alpha}=\pi N(\epsilon_{\alpha})|V_{kd}|^2{}_{\mathrm{AVE}}. \quad (2c)$$

Here $N(\epsilon_{\alpha})$ is the density of band states in the perfect crystal at energy ϵ_{α} and the matrix elements are averaged over k states of this energy.

If $\epsilon_+>0$ and $\epsilon_-<0$, then for $V_{kd}\to 0$ the ground state is given by the filled Fermi sea and a single electron occupying the d orbital. Since the states with d-electron spin $\uparrow$ and $\downarrow$ are degenerate, a localized moment occurs even at zero temperature in this case. For small but finite V_{kd}, i.e. $r_{\alpha}\ll 1$, these two spin states are mixed by electrons hopping on and off the d orbital, due to V. Under what conditions can this hopping quench the localized moment?

Unfortunately, this question cannot be answered by treating V directly by perturbation theory, since arbitrarily small energy denominators $\epsilon_k-\epsilon_{k'}\simeq 0$ enter in fourth and higher orders in V. However, one can isolate those interactions which dominate the dynamics of the system for $r_{\alpha}\ll 1$ by performing a canonical transformation which eliminates V_{kd} to first order. Thus, we require that

$$\bar{H}\equiv e^{S}He^{-S} \quad (3)$$

have no terms which are first order in V. If we denote the first three terms in H by H_0 and the term involving V by H_1, then by choosing S to be first order in V, one has

$$[H_0,S]=H_1, \quad (4)$$

and

$$\bar{H}=H_0+\tfrac{1}{2}[S,H_1]+\tfrac{1}{3}[S,[S,H_1]]+\tfrac{1}{8}[S,[S,[S,H_1]]]+\cdots. \quad (5)$$

From (4) one finds the generator S is given by[4]

$$S=\sum_{ks\alpha}\frac{V_{kd}}{\epsilon_k-\epsilon_{\alpha}}n_{d,-s}{}^{\alpha}c_{ks}{}^{+}c_{ds}-\mathrm{H.C.}, \quad (6)$$

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[1] P. W. Anderson, Phys. Rev. **124**, 41 (1961).

[2] J. Kondo, Progr. Theoret. Phys. (Kyoto) **32**, 37 (1964).

[3] H. Suhl, Phys. Rev. **138**, A515 (1965); Y. Nagaoka, *ibid.* **138**, A1112 (1965); A. A. Abrikosov, Physics **2**, 5 (1965); **2**, 61 (1965).

[4] It would appear that the singularity of S for states with $\epsilon_k\simeq\epsilon_{\alpha}$ leads to difficulties. By carrying out a similar analysis in a Green's-function scheme one finds that ϵ_k is replaced by a frequency variable ω, with the behavior near the pole being given by the analytic properties of the Green's functions. The situation is analogous to the Bardeen-Pines versus the Eliashberg elimination of the phonons in superconductivity. See J. R. Schrieffer, *Theory of Superconductivity* (W. A. Benjamin and Company, Inc., New York, 1964).

where the projection operators $n_{d,-s}{}^{\alpha}$ are defined by

$$n_{d,-s}{}^{\alpha}=n_{d,-s}, \quad \alpha=+; \qquad =1-n_{d,-s}, \quad \alpha=-. \tag{7}$$

While the transformed Hamiltonian (5) is complicated, we will see that in the limit $r_\alpha \ll 1$, $\bar{H}$ is well approximated by H_0+H_2, where

$$H_2=\tfrac{1}{2}[S,H_1]=H_{\rm ex}+H_{\rm dir}+H_0{}'+H_{\rm ch}. \tag{8}$$

These four terms can be expressed in terms of the field operators

$$\Psi_k=\begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} \quad \text{and} \quad \Psi_k=\begin{pmatrix} c_{d\uparrow} \\ c_{d\downarrow} \end{pmatrix}:$$

(a) an s-d exchange interaction,

$$H_{\rm ex}=-\sum_{kk'} J_{k'k}(\Psi_{k'}{}^{\dagger}\mathbf{S}\Psi_k)\cdot(\Psi_d{}^{\dagger}\mathbf{S}\Psi_d), \tag{9a}$$

where $2\mathbf{S}=\boldsymbol{\sigma}$ are the Pauli matrices and

$$J_{k'k}=V_{k'd}V_{dk}\{(\epsilon_k-\epsilon_+)^{-1}+(\epsilon_{k'}-\epsilon_+)^{-1} -(\epsilon_k-\epsilon_-)^{-1}-(\epsilon_{k'}-\epsilon_-)^{-1}\}; \tag{9b}$$

(b) a direct (i.e. spin independent) s-d interaction,

$$H_{\rm dir}=\sum_{kk'}\{W_{k'k}+\tfrac{1}{4}(J_{k'k})(\Psi_d{}^{\dagger}\Psi_d)\}(\Psi_{k'}{}^{\dagger}\Psi_k), \tag{10a}$$

where

$$W_{k'k}=\tfrac{1}{2}(V_{k'd}V_{dk})\{(\epsilon_k-\epsilon_-)^{-1}+(\epsilon_{k'}-\epsilon_-)^{-1}\}; \tag{10b}$$

(c) a term which we absorb into H_0 by shifting the definitions ϵ_+ and ϵ_-,

$$H_0{}'=-\sum_{k,s}\{W_{kk}+\tfrac{1}{2}J_{kk}n_{d,-s}\}n_{ds}; \tag{11}$$

(d) a term which changes the occupancy of the d orbital by two electrons,

$$H_{\rm ch}=\tfrac{1}{4}\sum_{kk's} J_{k'k}c_{k',-s}{}^{\dagger}c_{ks}{}^{\dagger}c_{ds}c_{d,-s}+\text{H.C.} \tag{12}$$

Since a localized moment is most likely to occur if $\epsilon_+>0$, $\epsilon_-<0$, we restrict the discussion to this case. Since all terms in H_2 conserve the number of d electrons except $H_{\rm ch}$, which changes the number by two, it follows that H_2 does not connect the part of Hilbert space having one d electron (the case of interest) with the remainder of Hilbert space, i.e., zero or two d electron states. Therefore $H_{\rm ch}$ can be neglected. Furthermore, in the one-d-electron subspace, $(\Psi_d{}^{\dagger}\Psi_d)=1$ so that $H_{\rm dir}$ reduces to a one-body potential which can be eliminated by transforming from the k states to a set of one-electron conduction states which include this direct scattering term. For $r_\alpha \ll 1$, the resultant shift of the conduction-electron wave functions and energies is negligible. Thus, H_2 reduces to the s-d exchange interaction (9). For k and $k'\simeq k_F$, $J_{kk'}$ is given by

$$J_{k_Fk_F}\equiv J_0=2|V_{k_Fd}|^2\frac{U}{\epsilon_d(\epsilon_d+U)}<0. \tag{13}$$

This coupling is antiferromagnetic, as was previously recognized.[5]

Were it not for the Kondo effect, H_2 could be treated by perturbation theory. As Kondo, Suhl, and Nagaoka[3] have pointed out, there is another dimensionless parameter $K\equiv N(0)J_0\ln(D/k_BT)$ which enters if $J_{kk'}$ is approximated by a constant in an energy interval $D(\sim\epsilon_\alpha)$ about the Fermi surface and zero outside this region. For $T<T_c=(D/k_B)e^{-1/N(0)J_0}$, K is larger than unity and perturbation theory breaks down. It appears that this breakdown corresponds to a condensation in which the conduction electrons develop a spin polarization in the vicinity of the impurity which is coupled with the localized impurity spin to form a state of total spin zero, i.e., the localized moment is quenched.[6]

In bringing about the condensation the most important virtually excited states are those of energy $|\epsilon_k|\gtrsim k_BT_c\ll|\epsilon_\alpha|$. Therefore, in estimating the effect of the higher commutators in $\bar{H}$ (5), one can set $\epsilon_k-\epsilon_\alpha\simeq\epsilon_\alpha$. Since the small denominators $\epsilon_k-\epsilon_{k'}$ which lead to the parameter K never enter these commutators, it seems clear that the higher commutators will only lead to weak renormalization effects, of order r_α, $r_\alpha{}^2$, etc. We conclude that the Anderson Hamiltonian can be replaced by the Hamiltonian of the s-d exchange model with an effective exchange interaction given by (9b), so long as $r_\alpha\ll 1$, i.e., $N(0)J_0\ll 1$.

A similar transformation can be carried out for the case of several d orbitals, the results of which will be reported elsewhere.[7]

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[5] P. W. Anderson and A. M. Clogston, Bull. Am. Phys. Soc. **6**, 124 (1961); J. Kondo, Progr. Theoret. Phys. (Kyoto) **28**, 846 (1962).

[6] This result is complementary to that of Schrieffer and Mattis, who found that in the limit of a small fraction of an electron or a hole on the impurity, on the average, the ground state exhibits no localized moment. See J. R. Schrieffer and D. C. Mattis, Phys. Rev. **140**, A1412 (1965). As in the present analysis, they found correlation effects suppress the moment predicted by the Hartree-Fock approximation.

[7] B. Mühlschlegel and J. R. Schrieffer (private communication).