Relation between the Anderson and Kondo Hamiltonians

J. R. Schrieffer*  
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania

and

P. A. Wolff  
Bell Telephone Laboratories, Murray Hill, New Jersey  
(Received 24 March 1966)

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 alloy1 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 \( J_{sd} \). Since the Kondo effect apparently arises, 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 \( J_{sd} \).

The Anderson Hamiltonian for a single localized orbital \( ^{1d}_d \) is

\[
H = \sum_{k} \epsilon_{k} n_{kd} + \sum_{k} \epsilon_{d} n_{dd} + U n_{dd} n_{dd} + \sum_{k} \{ V_{kd} c_{kd}^{\dagger} c_{kd} + V_{kd}^{*} c_{kd} c_{kd}^{\dagger} \},
\]

where \( \epsilon_{k} \) and \( \epsilon_{d} \) 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

\[
\gamma_{\pm} = \Gamma_{\pm} / |\epsilon_{\pm}|,
\]

where

\[
\epsilon_{\pm} = \epsilon_{d} + U, \quad \alpha = \pm;
\]

and

\[
\Gamma_{\pm} = \pi N(\epsilon_{d}) |V_{kd}|^2 \text{AVB}.
\]

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

If \( \epsilon_{d} > 0 \) and \( \epsilon_{< 0} \), then for \( V_{kd} \rightarrow 0 \) 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. \( r_{d} \ll 1 \), these two spin states are mixed by electrons hopping on and off the \( d \) orbital, due to \( U \). 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 \( \epsilon_{k} - \epsilon_{d} \ll 0 \) enter in fourth and higher orders in \( V \). However, one can isolate those interactions which dominate the dynamics of the system for \( r_{d} \ll 1 \) by performing a canonical transformation which eliminates \( V_{kd} \) to first order. Thus, we require that

\[
\widetilde{H} = e^{g} H e^{-g}
\]

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 \( V , H_{1} \), then by choosing \( S \) to be first order in \( V \), one has

\[
[H_{0}, S] = H_{1},
\]

and

\[
\widetilde{H} = H_{0} + \frac{1}{2} [S, H_{1}] + \frac{1}{2} [S, [S, H_{1}]] + \cdots.
\]

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

\[
S = \sum_{\epsilon_{k} \epsilon_{d}} \frac{V_{kd}}{\epsilon_{d} - \epsilon_{k}} n_{kd}^{\dagger} c_{kd} c_{kd}^{\dagger} - H.C.,
\]

* This work was supported in part by the National Science Foundation.


4 It would appear that the singularity of \( S \) for states with \( \epsilon_{d} = \epsilon_{k} \), leads to difficulties. By carrying out a similar analysis in a Green's-function scheme one finds that \( \epsilon_{d} \) is replaced by a frequency variable \( \omega \), 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 \( n_{d,-\alpha} \) are defined by

\[
\begin{align*}
n_{d,-\alpha} &= n_{d,-\alpha}, & \alpha &= -1, \\
n_{d,-\alpha} &= 1 - n_{d,-\alpha}, & \alpha &= +1.
\end{align*}
\]

(7)

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

\[
H_\alpha = \frac{1}{2} \left[ S, H \right] = H_{ex} + H_{dir} + H_\alpha^\prime + H_{ch}.
\]

(8)

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

\[
\Psi_k = \begin{pmatrix} c_{k,1} \\ c_{k,1} \end{pmatrix} \quad \text{and} \quad \Psi_\delta = \begin{pmatrix} c_{d,1} \\ c_{d,1} \end{pmatrix}:
\]

(a) an \( s-d \) exchange interaction,

\[
H_{ex} = -\sum_{kk'} J_{kk'} (\Psi_{k'}^\dagger \Sigma \Psi_\delta) \cdot (\Psi_\delta^\dagger \Sigma \Psi_{k'}),
\]

(9a)

where \( 2S = \sigma \) are the Pauli matrices and

\[
J_{kk'} = V_{kk'} V_{dd} \{(\epsilon_k - \epsilon_\delta)^{-1} + (\epsilon_{k'} - \epsilon_\delta)^{-1} - (\epsilon_k - \epsilon_\delta)^{-1} - (\epsilon_{k'} - \epsilon_\delta)^{-1}\};
\]

(9b)

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

\[
H_{dir} = \sum_{kk'} \left\{ W_{kk'} + \frac{1}{2} (J_{kk'}) (\Psi_\delta^\dagger \Sigma \Psi_{k'}) \cdot (\Psi_{k'}^\dagger \Sigma \Psi_{k'}) \right\},
\]

(10a)

where

\[
W_{kk'} = \frac{1}{2} (V_{kk'} V_{dd}) \{(\epsilon_k - \epsilon_\delta)^{-1} + (\epsilon_{k'} - \epsilon_\delta)^{-1}\};
\]

(10b)

(c) a term which we absorb into \( H_0 \) by shifting the definitions \( \epsilon_k \) and \( \epsilon_\delta \),

\[
H_\delta' = -\sum_{kk'} \left\{ W_{kk'} + \frac{1}{2} J_{kk'} n_{d,-\delta} \right\} n_{d,-\delta} + \frac{1}{2} \sum_{kk'} J_{kk'} c_{k,-\delta}^\dagger c_{k,-\delta} + \text{H.C.,}
\]

(11)

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

\[
H_{ch} = \frac{1}{2} \sum_{kk'} J_{kk'} c_{k,-\delta}^\dagger c_{k,-\delta} + \text{H.C.}
\]

(12)

Since a localized moment is most likely to occur if \( \epsilon_\delta > 0 \), \( \epsilon_\delta < 0 \), we restrict the discussion to this case. Since all terms in \( H_\delta \) conserve the number of \( d \) electrons except \( H_{ch} \) which changes the number by two, it follows that \( H_\delta \) 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 \( H_{ch} \) can be neglected. Furthermore, in the one-\( d \)-electron subspace, \( \langle \Psi_\delta c_{k,-\delta} \rangle = 1 \) so that \( H_{dir} \) 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 \( r_s \ll 1 \), 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 \( k' \approx k_F \), \( J_{kk'} \) is given by

\[
J_{kk'} = 2 |V_{kk'}|^2 \frac{U}{E_k (E_k + U)} < 0.
\]

(13)

This coupling is antiferromagnetic, as was previously recognized.\(^5\)

Were it not for the Kondo effect, \( H_0 \) could be treated by perturbation theory. As Kondo, Suhl, and Nagaoka\(^3\) have pointed out, there is another dimensionless parameter \( K = N(0) J_0 \ln (D/k_B T) \) which enters if \( J_{kk'} \) is approximated by a constant in an energy interval \( D (\sim \epsilon_\delta) \) 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.\(^4\)

In bringing about the condensation the most important virtually excited states are those of energy \( |\epsilon_k | > k_B T e^{-1/N(0)} \). Therefore, in estimating the effect of the higher commutators in \( \hat{H} \) (5), one can set \( \epsilon_k - \epsilon_\delta \approx \epsilon_\delta \). 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 \( r_s, r_s^2 \), 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 \( r_s \ll 1 \), i.e., \( N(0)/J_0 < 1 \).

A similar transformation can be carried out for the case of several \( d \) orbitals, the results of which will be reported elsewhere.\(^7\)


\(^6\) 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. Mühlechlegel and J. R. Schrieffer (private communication).