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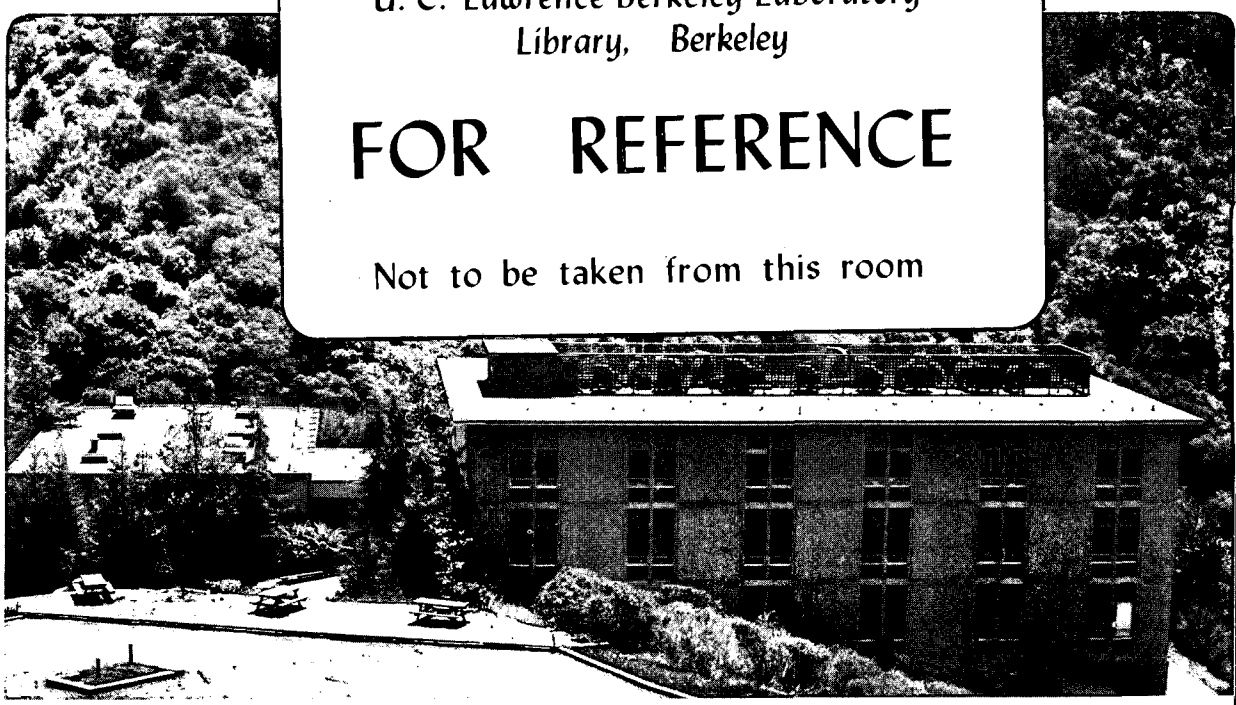

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SCHRIEFFER-WOLFF TRANSFORMATION OF THE LATTICE ANDERSON IMPURITY MODEL: LOCAL MOMENTS, KONDO LATTICE, HEAVY FERMIONS, INTERMEDIATE VALENCE, AND BAND THEORY

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ABSTRACT

The small-hybridization, large-coulomb-interaction regime of the lattice Anderson impurity model is studied by means of a canonical (Schrieffer-Wolff) transformation to determine the physical nature of the solutions. Emphasis is placed on the phenomenon of heavy fermions which occurs in the region where the Anderson model is mapped onto the large-interaction-strength limit of the Hubbard model ($t-J$ model).

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Crystalline compounds that involve lanthanide or actinide ions display a rich variety of physical phenomena: longe-range-ordered local magnetic moments[1] (ferromagnets, antiferromagnets, spiral or canted spin arrangements, *etc.*); Kondo lattices[2] (a strong interaction between conduction electrons and local moments that quenches the magnetic moments everywhere); heavy fermions[3,4] (materials characterized by a huge "density of states at the Fermi level"); intermediate valence[5] (strong charge fluctuations that produce [on average] only a fraction of an electron per ion); and band theory[6] (the electrons are approximated well by noninteracting particles).

Lanthanide and actinide compounds possess ions with localized (atomic) f-orbitals that do not overlap with the corresponding f-orbitals on neighboring ions, but do hybridize with the extended states of the conduction-band electrons. The f-electrons interact very strongly with each other via a screened (on-site) coulomb interaction U that acts only between two f-electrons that are localized about the same lattice site. The coulomb energy is larger than any other in the problem ($U > 10$ eV) so that double-occupied f-orbitals are effectively forbidden. The physics of such an electronic system is described by the lattice (or periodic) Anderson impurity model[7]

$$H_A = \sum_{k\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \varepsilon \sum_{i\sigma} f_{i\sigma}{}^\dagger f_{i\sigma} + U \sum_i f_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow}^\dagger f_{i\downarrow}$$

$$+ \sum_{ik\sigma} [V_{ik} f_{i\sigma}^\dagger a_{k\sigma} + V^*_{ik} a^\dagger_{k\sigma} f_{i\sigma}] \quad , \tag{1}$$

in the large-U ($U \to \infty$) limit.[8] The parameters and operators in Eq. (1) include the conduction-band creation (annihilation) operators $a^\dagger_{k\sigma}$ ($a_{k\sigma}$) for a conduction electron in an extended state with wavevector k, spin σ, and energy ε_k; the localized electron[9] creation (annihilation) operators $f^\dagger_{i\sigma}$ ($f_{i\sigma}$) for localized electrons in an atomic orbital centered at lattice site i with energy ε; the on-site coulomb interaction U; and the hybridization integral V_{ik} that mixes together the localized and extended states. The hybridization integral V_{ik} is assumed to be of the form

$$V_{ik} = \exp(i\mathbf{R}_i \cdot \mathbf{k})\, V\, g(k)/\sqrt{N} \quad , \tag{2}$$

with $g(k)$, the form factor, a dimensionless function of order one, and N the number of lattice sites. The Fermi level E_F is defined to be the maximum energy of the filled conduction band states, in the limit $V \to 0$, and the origin of the energy scale is chosen so that $E_F = 0$. The conduction-band density of states per site at the Fermi level is then defined to be ρ.

The lattice Anderson impurity model can be exactly diagonalized in two limits: in the noninteracting case ($U\rho \to 0$) the hamiltonian is a quadratic form in the fermionic operators, *i.e.* an independent particle problem, and can be diagonalized by a change in one-particle basis; in the zero hybridization limit ($V\rho \to 0$) the hamiltonian decouples into two independent systems (extended electrons and localized electrons), with explicitly diagonal subhamiltonians for each subsystem. The large-interaction ($U\rho \gg 1$), small-hybridization ($V\rho \ll 1$) limit of the Anderson model is the physically relevant regime for studying lanthanide and actinide compounds. Exact diagonalization studies[10] (on small systems) show that the lattice Anderson impurity model can describe all of the physical phenomena (local moments, Kondo effect, heavy fermions,

intermediate valence, and band theory) of lanthanide and actinide compounds simply by varying the parameter $\varepsilon\rho$ from large negative values to large positive values. In fact, the lattice Anderson impurity model, in the infinite-U and $V\rho \ll 1$ limit, is characterized by five regimes[8] depending upon the localized-electron energy ε (see Fig. 1):

(A) $\varepsilon\rho \ll -V\rho < 0$ — isolated local moments.[1] In this limit the f-orbitals are occupied by a single electron ($<f_{i\uparrow}^{\dagger} f_{i\uparrow} + f_{i\downarrow}^{\dagger} f_{i\downarrow}> = 1$), and (effectively) decoupled from the conduction electrons. There are everywhere local magnetic moments. The local moments interact with each other via exchange, superexchange, and/or Rudermann-Kittel-Kasuya-Yosida interactions[1] with ferromagnetic or antiferromagnetic exchange integrals.

(B) $-V\rho \ll \varepsilon\rho \ll -V^2\rho^2 < 0$ — the Kondo lattice.[2] In this regime there are no charge excitations in the localized orbitals ($<f_{i\uparrow}^{\dagger} f_{i\uparrow} + f_{i\downarrow}^{\dagger} f_{i\downarrow}> = 1$), but the local moments interact strongly with conduction-electron spins at the Fermi level to quench the magnetic moments everywhere.

(C) $\varepsilon\rho \approx -V^2\rho^2$ — the t–J model.[4] In this regime the localized orbitals are almost singly occupied ($<f_{i\uparrow}^{\dagger} f_{i\uparrow} + f_{i\downarrow}^{\dagger} f_{i\downarrow}> = 1-\nu$, $\nu \ll 1$) and have broadened into a strongly correlated narrow band in which all electronic transport takes place; the conduction band is (effectively) decoupled and acts only as a buffer that determines the concentration of electrons in the narrow band.

(D) $-V^2\rho^2 \ll \varepsilon\rho \ll V^2\rho^2$ — intermediate valence.[5] As ε is increased to the Fermi level and beyond the occupation of the localized orbitals becomes nonintegral ($0 < <f_{i\uparrow}^{\dagger} f_{i\uparrow} + f_{i\downarrow}^{\dagger} f_{i\downarrow}> < 1$) and the system is in the intermediate valence regime.

(E) $0 < V^2\rho^2 \ll \varepsilon\rho$ — band theory.[6] As ε is increased well beyond the Fermi level all localized states are unoccupied ($<f_{i\uparrow}^{\dagger} f_{i\uparrow} + f_{i\downarrow}^{\dagger} f_{i\downarrow}> = 0$) and (effectively) decoupled from the conduction electrons. The ground state is determined by one-

electron band theory for the extended electronic states.

Heavy-fermionic behavior[3,4] occurs, under certain circumstances, in regime (C), the transition region from the Kondo-lattice regime (B) to the intermediate-valence regime (D). The many-body ground state is characterized by a huge number of low-lying excited states that have many different spin configurations (a partial decoupling of spatial and spin degrees of freedom) and is close to a disproportionation instability. This produces a very large coefficient to the term linear in temperature in the specific heat, a large magnetic susceptibility, and poor metallic conductivity.

The five regimes outlined above may be established by employing a Schrieffer-Wolff[11] canonical transformation to the lattice Anderson impurity model. Since the details of this transformation are well known,[11,12] only an outline will be given here.

The Anderson hamiltonian H_A is divided into two terms $H_A = H_0 + H_{hyb}$ where H_{hyb} is the last term in Eq. (1). A canonical transformation $H' = \exp(S) H_A \exp(-S)$ is performed with S chosen to satisfy $[H_0, S] = H_{hyb}$. One finds (to lowest order in V) that $H' = H_0 + \frac{1}{2}[S, H_{hyb}]$ or

$$H' - H_0 = -\sum_{ikk'} J_{iikk'}\, \psi_{fi}^{\dagger} \boldsymbol{\sigma} \psi_{fi} \cdot \psi_k^{\dagger} \boldsymbol{\sigma} \psi_{k'} \tag{3a}$$

$$-\sum_{ii'k\sigma} [W_{ii'kk} + \frac{1}{4} J_{ii'kk}\, (f_{i\,-\sigma}^{\dagger} f_{i\,-\sigma} + f_{i'\,-\sigma}^{\dagger} f_{i'\,-\sigma})] f_{i\sigma}^{\dagger} f_{i'\sigma} \tag{3b}$$

$$+\sum_{ikk'} [W_{iikk'} + \frac{1}{4} J_{iikk'}\, \psi_{fi}^{\dagger} \psi_{fi}]\, \psi_k^{\dagger} \psi_{k'} \tag{3c}$$

$$+\frac{1}{4} \sum_{ikk'\sigma} [K_{iikk'}\, f_{i\sigma}^{\dagger} f_{i\,-\sigma}^{\dagger}\, a_{k\sigma} a_{k'\,-\sigma} + h.c.\,] \quad , \tag{3d}$$

where the spinors are defined to be

$$\psi_k \equiv \begin{bmatrix} a_{k\uparrow} \\ a_{k\downarrow} \end{bmatrix} \quad , \qquad \psi_{fi} \equiv \begin{bmatrix} f_{i\uparrow} \\ f_{i\downarrow} \end{bmatrix} \quad , \tag{4}$$

$\boldsymbol{\sigma}$ denotes the Pauli spin matrices, and the coefficients are

$$J_{ii'kk'} \equiv V_{ik} V^*_{i'k'} \left[\frac{1}{\varepsilon_k - \varepsilon - U} + \frac{1}{\varepsilon_{k'} - \varepsilon - U} - \frac{1}{\varepsilon_k - \varepsilon} - \frac{1}{\varepsilon_{k'} - \varepsilon} \right] , \tag{5a}$$

$$K_{ii'kk'} \equiv V_{ik} V_{i'k'} \left[\frac{1}{\varepsilon_k - \varepsilon - U} + \frac{1}{\varepsilon_{k'} - \varepsilon - U} - \frac{1}{\varepsilon_k - \varepsilon} - \frac{1}{\varepsilon_{k'} - \varepsilon} \right] , \tag{5b}$$

$$W_{ii'kk'} \equiv \tfrac{1}{2} V_{ik} V^*_{i'k'} \left[\frac{1}{\varepsilon_k - \varepsilon} + \frac{1}{\varepsilon_{k'} - \varepsilon} \right] . \tag{5c}$$

The last term (3d) can always be neglected (in the large-U limit) because it only connects configurations that have zero electrons at site i to configurations with two electrons at site i, which are explicitly forbidden.

The canonical transformation of the lattice Anderson impurity model is approximated well by the lowest order term (in V) when $|V^2\rho/\varepsilon| < 1$. In this region of parameter space the localized orbitals have an occupancy per site close to one ($\varepsilon < 0$) or close to zero ($\varepsilon > 0$). When the occupancy is close to one, the operator $\psi^\dagger_{fi} \psi_{fi}$ may be replaced by unity and both the term (3c) and the diagonal ($i = i'$) terms in (3b) may be absorbed into a renormalized H_0. The remaining terms in Eq. (3) describe spin scattering of the conduction electrons at the Fermi level by the localized moments (3a), and direct hopping terms within the (narrow) f-band (3b). When the occupancy is close to zero, the operators $\psi^\dagger_{fi} \psi_{fi}$, $\psi^\dagger_{fi} \boldsymbol{\sigma} \psi_{fi}$, and $f_i^\dagger f_{i'}$ may all be replaced by zero. The only important terms remaining in Eq. (3) are the changes in the one-particle band-structure arising from (3c).

The local-moment regime corresponds to the case where $\varepsilon\rho \ll -V\rho < 0$ so that $|J_{ii'kk'}| \ll 1$ for k and k' at the Fermi surface. To lowest order, the ground state consists of one f-electron per site and a conduction band filled up to energy E_F. The spin flipping of the local moments by the conduction-band electrons at the Fermi surface (3a) is weak and all other terms in Eq. (3) can be neglected.[13] The local moments interact with each other via all forms of exchange interactions, which determine, at low enough temperatures, the long-range magnetic order.

The Kondo lattice model corresponds to the case where $-V\rho \ll \varepsilon\rho \ll -V^2\rho^2 < 0$, the f-orbitals are singly occupied [so that the hopping term (3b) may be neglected], and the density of states of the conduction electrons is not negligible at the Fermi level, so that the spin scattering term (3a) is the most important correction term. The local-moment spins strongly interact with the conduction electrons (at the Fermi surface) which quench the magnetic moments everywhere.

The $t-J$ model occurs in the region where $\varepsilon\rho \approx -V^2\rho^2 < 0$. The localized states broaden into a narrow band with an occupancy of *nearly* one electron per site;[14] the density of states of the conduction electrons at the Fermi level is negligible, so that the spin-scattering term (3a) may be neglected. In this case, the hopping term (3b) is the most important correction term. The conduction electrons are decoupled from the f-band and act only as a buffer that determines the filling of the f-band. This narrow band is described by the large-U limit of the Hubbard model,[15] which becomes the $t-J$ model[16]

$$H_{t-J} = -\sum_{ij\sigma} t_{ij}\,(1-f_{i\,-\sigma}^{\dagger} f_{i\,-\sigma})\, f_{i\sigma}^{\dagger} f_{j\sigma}\,(1-f_{j\,-\sigma}^{\dagger} f_{j\,-\sigma}) + \sum_{ij} \mathrm{J}_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j \quad , \tag{6}$$

with

$$t_{ij} = \sum_k W_{ijkk} = \sum_k \frac{V_{ik}^{*} V_{jk}}{\varepsilon_k - \varepsilon} \quad , \tag{7}$$

and $\mathrm{J}_{ij} = 4\,|t_{ij}|^2/U$. Note that the hopping matrix elements t_{ij} in Eq. (7) are short-ranged, *i.e.*, strongly peaked functions of the separation $|\mathbf{R}_i - \mathbf{R}_j|$ between lattice sites i and j, as expected.

A necessary condition for heavy-fermion behavior is that the parameters of the Anderson model fall into the range where the mapping onto the $t-J$ model is valid, but this condition is not sufficient. The solutions of the $t-J$ model must also possess a very large number of low-lying excitations with many different spin configurations. This latter condition requires a *fine-tuning* of the parameters in the $t-J$ model and

depends strongly upon the geometry and connectivity of the lattice. For example, exact-diagonalization calculations on small clusters[17] indicate that strongly frustrated lattices, for occupancy close to one electron per site, are the best candidates for heavy-fermionic behavior (*e.g.*,the system with 7 electrons in an eight-site face-centered-cubic cluster possesses solutions with strongly enhanced low-temperature specific heat, quasielastic spin excitations, and poor metallic conductivity; the ground state may be magnetic or nonmagnetic).

The intermediate-valence regime occurs when the Schrieffer-Wolff transformation may not be truncated to lowest order, $|\varepsilon\rho| \ll V^2\rho^2$, or its expansion may not be valid at all. In this case, all parameters are equally important and the full many-body problem must be solved. The average occupation (per site) of an f-orbital decreases from 1 to 0 as $\varepsilon\rho$ is increased. This regime has been studied by mapping onto a Fermi liquid[5] and by exact-diagonalization on small clusters.[10]

Finally in the region where $\varepsilon\rho \gg V^2\rho^2$, the Schrieffer-Wolff transformation is once again valid to lowest order and one finds that the f-orbitals are completely empty and (effectively) decoupled from the conduction band. The system is described by one-electron theory[6] for the conduction-band electrons alone. This is the regime where ordinary density-functional theory is an excellent tool for calculating the electronic properties.

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$$\left| \frac{\sum_{FS} g^2(k)/\varepsilon}{\sum_{BZ} g^2(k)\exp(i\,\mathbf{k}\cdot\tau)/(\varepsilon_k-\varepsilon)} \right| \ll \nu \ll 1 \qquad ,$$

where τ is a nearest-neighbor translation vector, FS denotes a summation over wavevectors that lie on the Fermi surface only, and BZ denotes a summation over all wavevectors in the Brillouin zone.

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Figure Captions

Fig. 1. A schematic diagram showing the regions of parameter space where local magnetic moments, lattice Kondo effect (quenched moments everywhere), $t-J$ model, intermediate valence, and one-electron band theory are expected to occur in the small hybridization, large interaction strength limit of the lattice Anderson impurity model. The horizontal axis records the localized f-electron energy (relative to the Fermi level) and the vertical axis records the hybridization strength. Heavy-fermion behavior may occur in the transition region between the lattice Kondo effect and intermediate valence ($t-J$ model regime). A fine-tuning of the parameters and the crystal structure of the (effective) $t-J$ model is required to produce a heavy-fermion system.

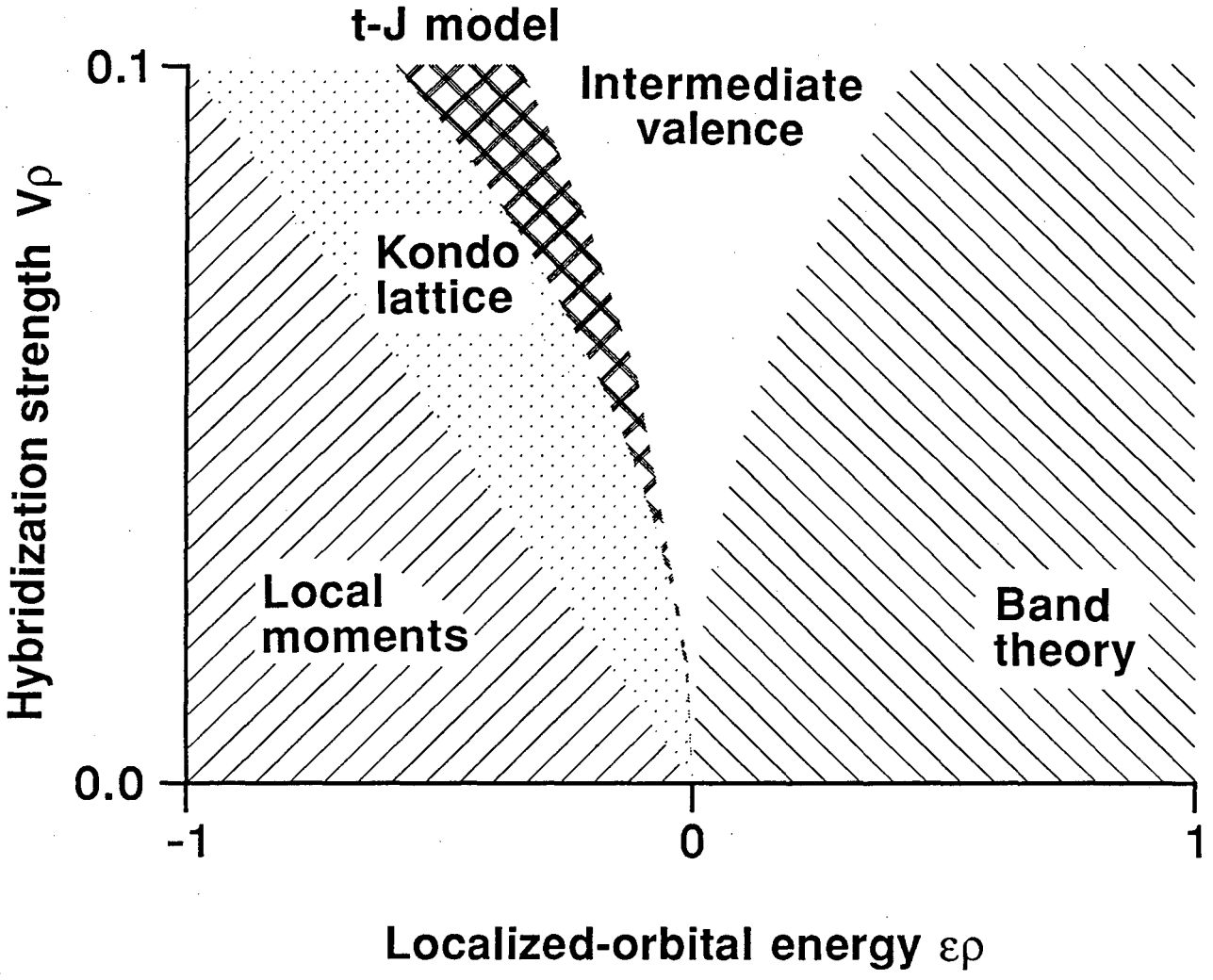
t-J model
0.1
0.0
Intermediate valence
Kondo lattice
Local moments
Band theory
Hybridization strength Vρ
-1
0
1
Localized-orbital energy ερ

FIGURE 1

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