# Gutzwiller method for heavy electrons

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The Kondo limit of the periodic Anderson model is studied with use of the Gutzwiller method. Because of the nonanalytic form of the energy gain due to hybridization, a small number of electrons are promoted out of the $f$-level giving rise to an almost-localized Fermi-liquid state of the $f$ electrons. Both symmetric and asymmetric limits of the Anderson model are discussed and in the former case the difference between the lattice and single-site problems is examined. A comparison is made to other examples of almost-localized Fermi liquids which are based on the Hubbard model. Finally the consequences of disorder in the Anderson model are examined.

## I. INTRODUCTION

The discovery that certain lanthanide and actinide intermetallic compounds have Fermi-liquid ground states rather than Ruderman-Kittel-Kasuya-Yosida- (RKKY) ordered antiferromagnetic ground states came as a surprise. Shortly after the first example $CeAl_3$, with its very large effective mass, was identified,[1] Mott[2] proposed that it belonged to the class of almost-localized Fermi liquids. This concept was introduced earlier by Brinkman and Rice[3] to describe the effect of the strong correlations on the metallic state close to the transition to the localized Mott insulating state. They applied their results to the metallic phase of $V_2O_3$ near the metal-insulator transition. Later Anderson and Brinkman[4] pointed out that the Fermi-liquid state of $^3$He had similar characteristics and recently Volhardt[5] gave an extensive discussion of the almost-localized model and its application to $^3$He. The discovery of superconductivity in some heavy-electron metals increased the interest in these materials[6] and an analogy between their properties and those of $^3$He was proposed by Anderson,[7] Ott *et al.*,[8] and Valls and Tesanovic.[9] In this paper we will examine this analogy using the Gutzwiller method, which allows us to make a direct comparison between the different systems that have been proposed as almost-localized Fermi liquids. Short accounts of part of this work have been published previously.[10]

The Gutzwiller method was formulated originally[11] for the Hubbard Hamiltonian. A clear exposition of the method was given by Vollhardt.[5] In Sec. II we follow his approach in our formulation of the method for the two-band Anderson lattice. In the Anderson model the number of electrons in the $f$ band is not fixed and is chosen to minimize the energy. This leads in general to two variational parameters representing the number of $f$ electrons and, when the on-site $f$-electron Coulomb repulsion $U$ is finite, the number of doubly occupied $f$-sites. The Gutzwiller method can also be used for a single-impurity Anderson model. There is a difference between the single-site and lattice models because in the first case the $f$ electron must return to the site it has left, whereas in the lattice problem $f$ electrons transfer between sites. We confine our attention to the Kondo limit where the $f$ level is well below the Fermi energy. An effective single-particle or renormalized-band Hamiltonian is obtained to describe the ground-state energy and its derivatives and the optimal choice of the parameters is determined variationally. Renormalized-band Hamiltonians have been obtained by a variety of methods and we refer the reader elsewhere for a review.[12] There are differences between our results and those obtained by other methods especially for small values of the $f$-level degeneracy $N_f$. The relationship of the present method to the other methods has been clarified in a forthcoming article by Kotliar and Ruckenstein[13] who have reformulated the Gutzwiller approximation in an elegant way as a particular mean-field theory using an auxiliary boson approach. We also should point out that there are two other papers on the Gutzwiller method for the Anderson model in our literature. Both have a basic similarity to our method although there are some differences in detail. Fazekas[14] concentrates on the mixed-valence regime and does not consider the Kondo limit of interest here. Varma, Weber, and Randall[15] present numerical results in the mixed-valence and Kondo limits. The overall results are similar but there seem to be some differences in detail that we will comment on below.

In Sec. III we present the results for two specific cases. First we study the symmetric Anderson Hamiltonian. In this case the number of $f$ electrons is exactly 1 but the nonanalytic form of the hybridization energy allows one to introduce a small number of holes and doubly occupied sites in the $f$ levels which are then optimized. In this case for a simple band structure the hybridization gap truncates the whole Fermi surface, and the ground state is in-

 

sulating and has no Pauli susceptibility. Secondly we study the asymmetric model in which the bare $f$ level is below the Fermi energy and the intrasite $f$-$f$ Coulomb repulsion $U\rightarrow\infty$. In this model we obtain a metallic state away from integral band filling. In both cases the ground-state energy has a Kondo-like form but the exponent differs from the single-site result for a finite value of $N_f$, the $f$-level degeneracy parameter. In the symmetric case this difference could be traced to the propagating terms that are present in the lattice problem but not in the single-site problem. In the asymmetric case the Fermi-liquid parameters may be determined. In our scheme the higher Fermi-liquid parameters ($F_l^{s,a}$; $l\geq 1$), as a consequence of the local character of the Fermi liquid, are simply zero.

In Sec. IV, we consider the effect of introducing disorder in the conduction band and in the $f$ levels. In the former case one can easily show that if one assumes a constant renormalization of the hybridization at all sites, then the effect of the disorder can simply be transformed away. In the case of $f$-level disorder this is not possible. However, the assumption of a site-independent renormalization is a severe one and we examine the conditions for it to be consistent. This problem has also been considered recently by Tesanovic.[16] He finds a stronger sensitivity to disorder than we do for disorder in the $f$ level.

Section V contains some concluding remarks on the relation of this heavy-electron problem to other systems that have been treated within the almost-localized-fermion approach.

## II. DERIVATION OF EFFECTIVE HAMILTONIAN

Our starting point is the periodic Anderson Hamiltonian which has the form

$$H=\sum_{k,\sigma}\varepsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}+\sum_{k,l,\sigma}V_{kl}(c_{k\sigma}^{\dagger}f_{kl\sigma}+f_{kl\sigma}^{\dagger}c_{k\sigma}) +E_f\sum_{i,l,\sigma}n_{il\sigma}+\tfrac{1}{2}U\sum_{\substack{i\\ l,\sigma\neq l',\sigma'}}n_{il\sigma}n_{il'\sigma'}\ , \tag{2.1}$$

where $n_{il\sigma}=f_{il\sigma}^{\dagger}f_{il\sigma}$ is the number operator for $f$ electrons at site $i$. The dispersion of the conduction electrons $\varepsilon_k$ is chosen to be linear and the band ranges $-1\leqq\varepsilon_k\leqq 1$. The $f$ level, $E_f$, is placed below the center of the conduction band so that the system is in the Kondo regime. The orbital degeneracy of the $f$ states is denoted by the $l$ quantum number ($l=1,\ldots,L$) with a total degeneracy of $N_f=2L$ (including spins). The mixing matrix element $V_{kl}$ is assumed to be local ($k$ independent).

As a variational wave function for the ground state we use a wave function of Gutzwiller's form. In the present two-band ($f$ and $c$ bands) model when one projects out the weight of doubly occupied $f$ states, then the total number of $f$ electrons diminishes. Therefore we need to specify the final number of $f$ electrons per site $n_f$, and to minimize the total energy with respect to $n_f$. The wave function is of the form

$$|\Psi\rangle=P_{n_f}P\,|\Psi_0\rangle\ , \tag{2.2}$$

where $P_{n_f}$ is the projection operator onto the subspace of a fixed $n_f$. $P$ is Gutzwiller's projection operator

$$P=\prod_i\left[1-(1-g)\sum_{l,\sigma\neq l',\sigma'}n_{il\sigma}n_{il'\sigma'}\right] \tag{2.3}$$

and $|\Psi_0\rangle$ is a ground-state wave function for $U=0$.

The ground-state energy is given by

$$E_g=\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}\ . \tag{2.4}$$

For the time being we assume no orbital degeneracy, $L=1$, but only the spin degeneracy. A generalization to an arbitrary $L$ is straightforward. Let $M$, $N_{f\uparrow}$ ($N_{f\downarrow}$), and $D$ be the number of lattice sites, singly occupied sites by $f$ electrons with up (down) spin, and doubly occupied sites. In the Gutzwiller method, the difficulty lies in the calculation of the expectation value of the kinetic energy term, in our case, the mixing term. The original method has been very much simplified by Ogawa, Kanda, and Matsubara[17] and by Vollhardt.[5] In their scheme we take into account the effect of the projection on the doubly occupied site by a simple classical statistical weight but maintain the quantum coherence of the phase of the wave function $|\Psi_0\rangle$. We denote the number of configurations with definite values of $N_{f\uparrow}$, $N_{f\downarrow}$, $D$ by

$$N_D(M,N_{f\uparrow},N_{f\downarrow})=\begin{bmatrix}M\\N_{f\uparrow}\end{bmatrix}\begin{bmatrix}N_{f\uparrow}\\D\end{bmatrix}\begin{bmatrix}M-N_{f\uparrow}\\N_{f\downarrow}-D\end{bmatrix}\ . \tag{2.5}$$

The normalization integral of the wave function is given by

$$\langle\Psi|\Psi\rangle=\sum_D g^{2D}N_D(M,N_{f\uparrow},N_{f\downarrow})P(M,N_{f\uparrow}) \times P(M,N_{f\downarrow})\ , \tag{2.6}$$

where

$$P(M,N_{f\sigma})=n_{f\sigma}^{N_{f\sigma}}(1-n_{f\sigma})^{M-N_{f\sigma}}\ , \tag{2.7}$$

with $n_{f\sigma}=N_{f\sigma}/M$, is just the statistical weight neglecting any spatial correlation. By using the dominant-term approximation[5] for the sum $\sum_D$, we get the relation between the original variational parameter $g$ and the fraction of the doubly occupied sites $d=D/M$, which we will use as a variational parameter,

$$g^2=\frac{d(1-n_f-d)}{(n_{f\uparrow}-d)(n_{f\downarrow}-d)}\ . \tag{2.8}$$

The difference from the Hubbard model is the existence of the mixing terms. With the assumption of a $k$-independent $V$ we can use the site representation. The average for the mixing term from the $f$ to the $c$ state is

$$\langle\Psi|c_{i\sigma}^{\dagger}f_{i\sigma}|\Psi\rangle=\sum_{D}g^{2D}[N_D(M-1,N_{f\sigma}-1,N_{f\bar{\sigma}})+gN_D(M-1,N_{f\sigma}-1,N_{f\bar{\sigma}}-1)]\times P(M-1,N_{f\sigma}-1)P(M,N_{f\bar{\sigma}})\times\langle\Psi_0|c_{i\sigma}^{\dagger}f_{i\sigma}|\Psi_0\rangle\ , \tag{2.9}$$

where $\bar{\sigma}$ denotes the spin opposite to $\sigma$.

By using the dominant-term approximation again we get

$$\frac{\langle\Psi|c_{i\sigma}^{\dagger}f_{i\sigma}|\Psi\rangle}{\langle\Psi|\Psi\rangle}=q_{1\sigma}\langle\Psi_0|c_{i\sigma}^{\dagger}f_{i\sigma}|\Psi_0\rangle\ , \tag{2.10}$$

where the renormalization factor for the vertex is

$$q_{1\sigma}=\frac{1}{n_{f\sigma}}\left[(n_{f\sigma}-d)+g\frac{(n_{f\sigma}-d)(n_{f\bar{\sigma}}-d)}{1-n_f+d}\right]\ . \tag{2.11}$$

The first term in the large parentheses corresponds to the process of Fig. 1(a) and the second term to Fig. 1(b). On the other hand for the transfer from $c$ to $f$ states, the renormalization factor of $q_{2\sigma}$ defined by

$$\frac{\langle\Psi|f_{i\sigma}^{\dagger}c_{i\sigma}|\Psi\rangle}{\langle\Psi|\Psi\rangle}=q_{2\sigma}\langle\Psi_0|f_{i\sigma}^{\dagger}c_{i\sigma}|\Psi_0\rangle \tag{2.12}$$

is

$$q_{2\sigma}=\frac{1}{1-n_{f\sigma}}[(1-n_f+d)+g(n_{f\bar{\sigma}}-d)]\ . \tag{2.13}$$

The process shown in Fig. 1(c) contributes the first term in the brackets, while that in Fig. 1(d) gives the second.

In the evaluation of the energy, these two vertices appear always in pairs. Therefore the final result can be expressed by an expectation value

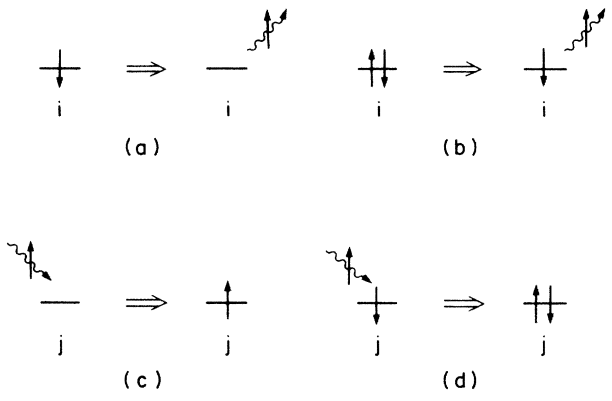


FIG. 1. Illustration of the four possible transitions: (a) and (b), removal of $f$ electron from site $i$; (c) and (d), addition of $f$ electron at site $j$.

$$E_g=\langle\Psi_0|H_{\rm eff}|\Psi_0\rangle+Ud \tag{2.14}$$

of the effective Hamiltonian with a fixed $n_{f\sigma}$,

$$H_{\rm eff}(n_{f\sigma})=\sum_{k,\sigma}\varepsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}+E_f\sum_{i,\sigma}n_{i\sigma}+\sum_{i,\sigma}Vq_{\sigma}^{1/2}(n_{f\sigma})(c_{i\sigma}^{\dagger}f_{i\sigma}+f_{i\sigma}^{\dagger}c_{i\sigma})\ , \tag{2.15}$$

where the renormalization factor is given by

$$q_{\sigma}(n_{f\sigma})=q_{1\sigma}q_{2\sigma}=\frac{1}{n_{f\sigma}(1-n_{f\sigma})}\{(n_{f\sigma}-d)(1-n_f+d)+(n_{f\bar{\sigma}}-d)d+2[(n_{f\sigma}-d)(n_{f\bar{\sigma}}-d)d(1-n_f+d)]^{1/2}\}\ . \tag{2.16}$$

The renormalization factor $q_{\sigma}$ is identical to that obtained for the Hubbard model and used previously.[10]

There are two typical cases which are of interest. One is the symmetric case $E_f+U=-E_f$, a symmetric conduction band, and the total number of electrons per site $n=2$. In this case the number of $f$ electrons is precisely one per site, and it is essential to keep $U$ finite. The other is an asymmetric case: $E_f+U>|E_f|$, where the number of $f$ electrons per site is slightly less than one. For the latter case we can take the limit of $U\to\infty$, but the degeneracy of the $f$ states is important as we will see below. It is straightforward to generalize the present method to the asymmetric case and to include orbital degeneracy. The result is a trivial extension of the effective Hamiltonian including the orbital degeneracy with a renormalization factor for $d=0$ ($U\to\infty$) (Ref. 10)

$$q_{\sigma}(n_{fl\sigma})=\frac{1-n_f}{1-n_{fl\sigma}}\ . \tag{2.17}$$

## III. GROUND-STATE AND LANDAU PARAMETERS

### A. Condensation energy and relation to Kondo energy

First we discuss the symmetric case. Instead of fixing $n_{f\sigma}$ we can go over to the equivalent of a grand canonical ensemble by introducing a Lagrange multiplier or a "chemical potential" $\mu_{\sigma}$, leading to an effective Hamiltonian

$$K_{\rm eff}=H_{\rm eff}-\sum_{i,\sigma}\mu_{\sigma}f_{i\sigma}^{\dagger}f_{i\sigma}\ . \tag{3.1}$$

The Hamiltonian can be diagonalized at once, giving hybridized bands

$$\xi_{k,\pm\sigma}=\tfrac{1}{2}\{\varepsilon_k+E_f-\mu_{\sigma}\pm[(\varepsilon_k-E_f+\mu_{\sigma})^2+4\tilde{V}_{\sigma}^2]^{1/2}\}\ , \tag{3.2}$$

where $\tilde{V}_{\sigma}^2=q_{\sigma}(n_{f\sigma})V^2$. The $+$ ($-$) label refers to the upper (lower) hybridized band. We consider the paramagnetic case. For the symmetric case, $n=2$ so that the

lower band is filled leaving the upper band empty. The number of $f$ electrons is given by

$$n_f=\frac{1}{M}\sum_{k,\sigma}\left[\frac{(\varepsilon_k-E_f+\mu)}{2[(\varepsilon_k-E_f+\mu)^2+4\tilde{V}^2]^{1/2}}+\frac{1}{2}\right]. \quad (3.3)$$

The condition of $n_f=1$ is satisfied by putting the effective $f$ level at the middle of the conduction band, i.e., $E_f-\mu=0$.

The expression for the ground-state energy reduces to

$$E_g=-\tfrac{1}{2}(1+4\tilde{V}^2)^{1/2}+2\tilde{V}^2\ln\tilde{V}+dU\ , \quad (3.4)$$

with the renormalization factor $q=8d$. By minimizing with respect to $d$, we get

$$d=\frac{1}{8V^2}e^{-(U/8V^2)} \quad (3.5)$$

and the final result for the ground-state energy is

$$E_g=-\tfrac{1}{2}-2e^{-(U/8V^2)}\ . \quad (3.6)$$

The binding energy has a Kondo form but the exponent is a factor of 2 smaller than the single-site Kondo problem,[18]

$$T_K=2\exp(1/J_K\rho)=2\exp(-U/4V^2)\ .$$

In the Gutzwiller method, we neglect spatial correlations in the evaluation of the statistical weight. In the lattice problem we may justify the approximation on the basis that the processes of hopping out from and into $f$ shells are slow processes and between those processes the electron migrates to many sites as a conduction electron. On the other hand for the single-site problem, the process of Fig. 1(a) should be accompanied by (c) and (b) by (d) since these processes can take place only on one site. The combination of (a) and (d) or (b) and (c) is allowed only for pairs of different sites and so can occur in the lattice problem. Therefore the renormalization factor for the symmetric single-site problem should be modified to

$$q=4d\ , \quad (3.7)$$

leading to the correct binding energy of the single-site Kondo problem quoted above.

Next we consider the asymmetric case. By changing the electron number from the half-filled case we can have a metallic ground state. We consider the case of $n=1+\varepsilon_0$ $(0<\varepsilon_0<1)$. After similar calculations as in the symmetric case, we obtain[10]

$$E_g=-\tfrac{1}{2}[1-(\varepsilon_0-1)^2]+E_f-\varepsilon_0\exp\left[-\frac{2L-1}{2L}\frac{\varepsilon_0-1-E_f}{LV^2}\right]. \quad (3.8)$$

The quasiparticle hybridized bands are shown in Fig. 2. The binding energy has a Kondo form again. The exponent coincides with the single-site case in the large-degeneracy limit ($L\to\infty$), but differs by a factor of 2 for the orbitally nondegenerate case ($L=1$).

The $f$-band occupancy is slightly less than one,

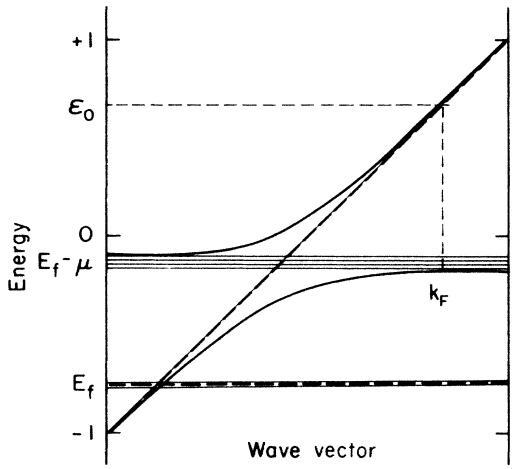


FIG. 2. Schematic band structure illustrating the bare conduction band of width 2, center 0, the bare $f$ bands at energy $E_f$, and the hybridized quasiparticle bands. $k_F$ is the Fermi wave vector corresponding to a density of electrons $n$ (i.e., including $f$ electrons), $\varepsilon_0$ is the conduction-band energy $\varepsilon(k_F)$, and the density of $f$ electrons $n_f\lesssim 1$.

$$1-n_f=\frac{2L-1}{2L}\frac{\varepsilon_0}{LV^2}\exp\left[-\frac{2L-1}{2L}\frac{\varepsilon_0-1-E_f}{LV^2}\right]. \quad (3.9)$$

It should be noted that the deviation of $n_f$ from one is nonanalytic with respect to $V$. It arises from a balance between a large positive term proportional to $(1-n_f)$ which represents the energy cost to promote an electron from the bare $f$ level to the Fermi level and a negative term proportional to $(1-n_f)\ln(1-n_f)$ which represents the energy gain from the formation of the hybridized bands. As a result a value of $n_f<1$ occurs for all values of $V$ and $E_f$. We note that a transition to a value $n_f=1$ was reported in numerical calculations by Varma *et al.*[15] as $E_f$ moves well below the Fermi energy in a paramagnetic state; however, in our analytic result this does not happen. There can be a magnetic transition which leads to $n_f\to 1$, as we discuss below.

### B. Landau parameters

For the metallic ground state of the asymmetric case, we can discuss Landau Fermi-liquid parameters, and the low-lying excitations.

The specific heat is given by the density of quasiparticle states

$$N_0=\frac{(\varepsilon_0-E_f+\mu)^2}{qLV^2}=\frac{1}{qLV^2}\ . \quad (3.10)$$

Since it involves $q^{-1}$, as expected, it can be very large. The denominator corresponds to an effective Fermi temperature or Kondo binding energy.

It is straightforward to calculate the charge susceptibility $\chi_c$ which is determined by the shift in the chemical potential due to a change in the total number of electrons $n$ or equivalently $\varepsilon_0$. A change in $\varepsilon_0$ hardly changes $n_f$, and

the hybridized quasiparticle bands ride with $\varepsilon_0$. As a result the total charge susceptibility $\chi_c$ is that of the conduction band and the parameter $F_0^s$ must be very large since it must cancel the large effective-mass term. We find[10]

$$\chi_c = 1 \quad \text{and} \quad F_0^s \cong (qLV^2)^{-1} . \tag{3.11}$$

The positive sign of $F_0^s$ also shows that there remains strong residual repulsive interactions between quasiparticles which will tend to suppress conventional $s$-wave superconductivity.

The magnetic susceptibility, $\chi_s$ is obtained by taking the second derivative of the energy with respect to the magnetization $m$. Since the renormalization factor $q_\sigma$ is sensitive to $m$ through the denominator in Eq. (2.17), there is an important interaction correction. Using simply a constant $g$ factor for all values of $l$ and neglecting any orbital moment leads to a Wilson ratio

$$\frac{\chi_s}{N_0} = \left[ 1 - \frac{4L-3}{(2L-1)^2} - \frac{2L}{(2L-1)^2} \ln \left[ \frac{\varepsilon_0}{qLV^2} \right] \right]^{-1}$$

$$= (1+F_0^a)^{-1} . \tag{3.12}$$

If $L=1$ (only spin degeneracy), $\chi_s < 0$ always or the paramagnetic state is unstable towards magnetic ordering in the Kondo limit that we consider. The present treatment covers only a uniform magnetic state. The actual magnetic order will of course be determined by the detailed structure of the conduction band and the resulting Ruderman-Kittel-Kasuya-Yosida interaction. If the orbital degeneracy is large the paramagnetic state can be stable even in the Kondo regime where the effective mass is large. The condition is

$$2L \geq \frac{(\varepsilon_0 - E_f - 1)}{LV^2} \tag{3.13}$$

when Eq. (3.9) is used to rewrite the logarithmic term. The quantity $(\varepsilon_0 - E_f - 1)$ is the depth of the bare $f$ level from the Fermi energy and $\frac{1}{2}\pi LV^2$ is the width of the virtual level in the single-site problem. This ratio governs the crossover between Kondo and mixed-valence regimes. A similar conclusion, that the orbital degeneracy is essential to stabilize the paramagnetic state, has been reached using different methods by Coleman,[19] Read *et al.*,[20] and Yamada *et al.*[21]

Lastly we turn to other Landau parameters. It has been pointed out by several authors[22–25] that momentum dependence of the interaction effect may not be important. In our scheme the renormalization procedure is also essentially local and the renormalization factor $q$ is a function only of the average occupation numbers. Therefore if we make distortions of the Fermi surface corresponding to displacements in $\mathbf{k}$ space, higher-order spherical harmonics, etc., which do not change the average numbers then there are no interaction effects beyond the superposition of quasiparticles and so higher Landau Fermi-liquid parameters are zero in the present scheme. Presumably in a more realistic scheme they could take small values which are necessary to satisfy the forward scattering amplitude sum rule. In the one-band Hubbard model it can be shown quite generally that $F_1^{s,a}$ are small in the almost-localized limit.[26]

The fact that the term $F_1^s$ is zero (or small) means that the effective number of carriers is small, in fact $\propto (1-n_f)$. The effective number of carriers enters the plasma frequency of the Fermi liquid, $\omega_p$ and if $F_1^s \simeq 0$ then $\omega_p^2 \propto n/m^* \propto (1-n_f)/m$. Therefore we can interpret the effective carriers as holes in the $f$ band and the large effective mass as a way of reconciling the small number of effective carriers $1-n_f$, with the large number of carriers $n$. Note the Fermi surface contains $n$ the total number of electrons—conduction plus $f$ electrons—and at the Fermi energy the quasiparticle bands (in Fig. 2) have predominantly $f$ character. Therefore the simplest interpretation of the quasiparticles is that they are $f$ electrons whose enhanced mass reflects their almost-localized and strongly correlated character and the fact that they need to find an $f$ hole to move. Recent experiments[27] on the plasma frequency of the Fermi-liquid state in $UPt_3$ imply a small value for $F_1^s$ in agreement with the above discussion.

## IV. EFFECT OF DISORDER ON THE HEAVY-ELECTRON FERMI LIQUID

It is a remarkable experimental fact that small amounts of disorder on either the lanthanide/actinide lattice or in the conduction band have a dramatic effect on the coherence.[28] Indeed it often takes only a few percent of impurities and the resistivity no longer drops dramatically as $T \to 0$ K and the coherent ground state is apparently destroyed. Now one can write quite generally the dc conductivity as[2]

$$\sigma = \tfrac{2}{3} e^2 S_F \mathscr{L} / (2\pi)^3 , \tag{4.1}$$

where $S_F$ is the Fermi-surface area and $\mathscr{L}$ is the mean-free path. Now the area of the Fermi surface $S_F$ by Luttinger's theorem that the volume enclosed is related to the density of electrons, cannot vary appreciably so that the dramatic drop in the dc conductivity at $T=0$ K must come from a dramatic drop in $\mathscr{L}$, from values $\mathscr{L} \gg a$ to values $\mathscr{L} \sim a$. But this poses a serious problem since the mean-free path is not renormalized by the large mass enhancement and should be determined essentially by the spacing between impurities. However, for dilute concentrations the interimpurity spacing is much greater than $a$, hence an apparent paradox. This paradox was already recognized in the case of the first almost-localized Fermi liquid, namely, the metallic state of $V_2O_3$.[29] The only solution to the paradox is if the Fermi liquid itself is unusually sensitive to small disruptions of the coherence.

We consider then adding a disorder term to the periodic Anderson Hamiltonian

$$H_{\text{dis}} = \sum_{\substack{i \in \mathscr{S} \\ \sigma}} W_{fi} f_{i\sigma}^\dagger f_{i\sigma} + \sum_{\substack{i \in \mathscr{S} \\ \sigma}} W_{ci} c_{i\sigma}^\dagger c_{i\sigma} , \tag{4.2}$$

where $\mathscr{S}$ denotes the set of the sites with impurities and the potentials $W_f$ and $W_c$ act on the $f$ electrons and the conduction electrons, respectively. For simplicity we neglect the orbital degeneracy in this section $L=1$. A

similar model has been considered by Tesanovic.[16]

We start from a mean-field treatment of the impurity scattering. The critical strength for losing the coherence is given by a very simple argument. The ground-state energy for the asymmetric case as a function of $n_f$ is given by

$$E_g=\tfrac{1}{2}\varepsilon_0^2+(E_f-\varepsilon_0)n_f+\tfrac{1}{2}n_f^2 -\tfrac{1}{2}-qV^2\ln(\varepsilon_0/\omega_c)\ , \tag{4.3}$$

where the lower cutoff $\omega_c$ is $\omega_c=qV^2$ for the pure case. With impurities the inverse lifetime $\tau^{-1}=\frac{1}{2}(\tau_c^{-1}+\tau_f^{-1})$ plays the role of the cutoff. Now taking the derivative of $E_g$ with respect to $n_f$ at $n_f=1$ we get

$$\left.\frac{\partial E_g}{\partial n_f}\right|_{n_f=1}=E_f-\varepsilon_0+1+2V^2\ln(\varepsilon_0\tau)\ . \tag{4.4}$$

If the slope is positive then $n_f<1$ leads to $q\neq 0$ and therefore the system gains some energy by the coherent hybridization process. The critical strength in terms of the lifetime is

$$(\tau^{-1})_{\rm crit}=T_K\{=\varepsilon_0\exp[-(\varepsilon_0-1-E_f)/2V^2]\}\ . \tag{4.5}$$

However, the mean-field treatment overestimates the effect of the impurities giving a too stringent criterion for coherence.

Let us consider the effect of the disorder in the conduction band. In this case the part of the Hamiltonian involving only the conduction electrons is

$$H_{\rm cond}=\sum_{\mathbf{k},\sigma}\varepsilon(\mathbf{k})c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+\sum_{\substack{i\in\mathscr{S}\\ \sigma}}W_{c_i}c^\dagger_{i\sigma}c_{i\sigma}\ . \tag{4.6}$$

This can in general be diagonalized by a transformation to a new basis set of extended wave functions if $|W_c|\ll 1$. Let us denote the new basis by $\{\phi_n(\mathbf{r})\}$ and the new operators by

$$c^\dagger_{n\sigma}=\sum_i\phi_n^*(\mathbf{r}_i)c^\dagger_{i\sigma}\ . \tag{4.7}$$

Since the $f$ states are dispersionless we can make a corresponding transformation on the $f$ states and define

$$f^\dagger_{n\sigma}=\sum_i\phi_n^*(\mathbf{r}_i)f^\dagger_{i\sigma}\ . \tag{4.8}$$

The hybridization terms in the new basis is again (in the simplest (on-site) hybridization approximation] diagonal

$$\sum_{i,\sigma}V(f^\dagger_{i,\sigma}c_{i,\sigma}+\text{H.c.})=\sum_{n,\sigma}V(f^\dagger_{n\sigma}c_{n\sigma}+\text{H.c.})\ . \tag{4.9}$$

Therefore if we make a uniform renormalization of the hybridization $q(n_{f\sigma})$, i.e., independent of the site label $i$, then the effective Hamiltonian $H_{\rm eff}$ can be diagonalized and there is no change in the hybridization energy gain. As in Eq. (4.3) it will be proportional to $qV^2\ln(qV^2)$ and the only change that arises comes through the change in the conduction-band density of states. However, for weak scattering ($|W_c|\ll 1$) the change in the density of states is negligibly small and so we conclude that within the constant renormalization approximation, the renormalization factor would be unaffected by disorder in the conduction band. This agrees with the mean-field results of Tesanovic[16] who considered the same model. Note there is no assumption here of Bloch coherence.

However, the problem here is the assumption of the constant renormalization independent of the site. In the presence of impurity potentials the number of the $f$ electrons is no longer constant but fluctuates from site to site. We can estimate the fluctuation in the following way. Let us define a local off-diagonal charge susceptibility $\chi_c^{fc}$ which can be obtained from Eq. (3.9) as

$$\chi_c^{fc}=\frac{1}{2V^2}\exp\left[-\frac{\varepsilon_0-1-E_f}{2V^2}\right]=\frac{1}{\varepsilon_0}\frac{T_K}{2V^2}\ . \tag{4.10}$$

Note that if we change energy of the conduction-band center at some site by $W_c$ it will change the cutoff energy $\varepsilon_0$ but not the argument of the exponent. The numerator in the exponent is the depth of the $f$ level measured from the chemical potential but this stays constant even if an energy $W_c$ is added. Now we demand that the fluctuation of the number of $f$ electrons

$$\{n_i|\chi_c^{fc}W_c|^2\}^{1/2}$$

should be less than $1-n_f=T_K/2V^2$, leading to the criterion of the coherence

$$(\tau_c^{-1})_{\rm crit}=\varepsilon_0\ , \tag{4.11}$$

where $\tau_c^{-1}=n_i|W_c|^2/\varepsilon_0$ and $n_i$ is the impurity density.

On the other hand when the disorder is on the $f$ electrons the relevant charge susceptibility is the diagonal one given by

$$\chi_c^{ff}=-\frac{\partial n_f}{\partial E_f}=\frac{1}{2V^2}\left[\frac{T_K}{2V^2}\right]\ . \tag{4.12}$$

Then the criterion is

$$(\tau_f^{-1})_{\rm crit}=2V^2\ \text{ or }\ \sqrt{n_i}\,|W_f|=2V^2\ , \tag{4.13}$$

where $\tau_f^{-1}=n_i|W_f|^2/2V^2$. This criterion disagrees with the results of Tesanovic.[16] In his calculation all the disorder in $E_f$, the bare $f$ level, appears in the renormalized level, $E_f-\mu$, i.e., $\mu$ is fixed unlike our calculation where $\mu$ varies from site to site in the presence of the disorder.

The criteria are much weaker than the mean-field result. The conclusion that potential disorder on the conduction or $f$-electron energies does not have a drastic effect is in agreement with that reached earlier by Fukuyama.[24] There remains the effect of disorder on the hybridization matrix element $V$. In the present theory it is clear that this disorder would also be renormalized by the $q$ factor (a point which Fukuyama also agrees to[30]), but nevertheless since the hybridization band gap is sensitive to the hybridization strength the states at the hybridization band edge could become localized as a result of such disorder, relatively easily, leading to a drastic effect on the transport properties. Such problems require further study.

## V. CONCLUSIONS

The model of almost-localized Fermi liquid was developed initially[3] for systems which are described by a

Hubbard Hamiltonian. In such systems the number of electrons per site is fixed and is usually integral. The band filling of the strongly correlated band is given. The almost-localized state is achieved only close to the critical boundary separating localized from itinerant behavior. In the case of the metallic state of $V_2O_3$ (Ref. 3) this boundary separates at low temperatures an insulating antiferromagnetic (AF) ordered state from the Fermi liquid and in liquid $^3$He (Refs. 4 and 5) it is the boundary to the crystalline state. The small parameter which leads to a small number of effective carrires and hence to a large mass, is the closeness to the critical boundary.

The heavy-electron metals are described by the two-band Anderson model and do not have a fixed number of electrons in the strongly correlated $f$ band. The small parameter originates in the weakness of the hybridization process. This ensures the smallness of the density of effective carriers [$d$ in the symmetric model, $(1-n_f)$ in the asymmetric limit]. There is no obvious inherent limit to the size of $d$ or $(1-n_f)$ and therefore to the mass enhancement which varies as $d^{-1}$ or $(1-n_f)^{-1}$. The competition to the localized state is represented here by the competition to the RKKY AF ordered state. In the Hubbard model the closeness to criticality that can be achieved before the onset of localization is strongly influenced by the crystal structure and the resultant band structure. Presumably here also the crystal structure plays a role but the precise factors which govern the choice between the RKKY and heavy-electron states remain open. Clearly a generalization to a more realistic treatment of crystal structure, and spin-orbit and crystal-field effects is required.

The relationship of the Gutzwiller approximation to the auxiliary boson and other methods developed for the heavy-electron problem has been clarified greatly by the very recent work of Kotliar and Ruckenstein.[13]

In conclusion we make a few comments on the physical interpretation of the heavy-electron state. The approach presented here is directly based on the Anderson Hamiltonian without making the Schrieffer-Wolff transformation to the Kondo Hamiltonian. The heavy-electron Fermi liquid arises through the introduction of a small number of holes (and also doubly occupied sites at finite $U$) into the $f$ band enabling a hybridized band state to occur. This introduces charge degrees of freedom in the $f$ band so that the density of states for electron-hole excitations in the $f$ band extends down to zero energy. Therefore in a band description of the Fermi liquid the $f$ band must appear at the Fermi energy and the Fermi surface must contain the $f$-electron states. In the localized RKKY state the $f$ bands have no low-lying charge degrees of freedom and the Fermi surface contains only the conduction states. This difference is, in principle, measurable, e.g., for a Ce compound with an odd number of Ce atoms in the unit cell.

Lastly we comment on the question of the nature of heavy electron. In our description the simplest interpretation is that heavy electrons are $f$ electrons. It is clear from Fig. 2 that the quasiparticle states have predominantly $f$ character at the Fermi energy. Further the large electronic entropy at low temperature that is implied by the large specific heat is clearly due to the $f$-spin degrees of freedom and there is a large number of $f$ electrons (e.g., $\simeq$ one per Ce atom). They move very slowly because of the very small number of empty (and doubly occupied) sites which is one way of looking at their heavy mass. Alternatively their characteristic Fermi temperature is very low and so their spin degrees of freedom have a very low characteristic energy and hence lead to a large linear specific heat as $T\rightarrow 0$ K. So we conclude that the heavy electrons are simply strongly correlated $f$ electrons.

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