Correlated Fermi-Liquid State Formed with Overlapping Kondo Clouds

—— *A Variational Study*[*] ——

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A simple variational description is given on the nature of overlapping Kondo clouds, which compensate the localized f-spins in the Kondo lattice. It is shown explicitly that the f-electrons participate in forming a "large Fermi surface", although they are strictly localized. The resulting correlated Fermi liquid, i.e., heavy fermions, is examined with the variational Monte Carlo method and is compared with the Gutzwiller approximation. The relation to the periodic Anderson model is also discussed in this connection.

§ 1. Introduction

Notwithstanding much efforts over more than 10 years, physics of heavy fermions is still far from well understood.[1)~3)] Experimentally, in addition to superconductivity magnetic properties of heavy fermions appear to be extremely complicated and challenging. Furthermore it is often a matter of controversy in what situation the f-electrons participate in forming the Fermi surface (i.e., "small" vs "large" Fermi surface). Theoretically, the basic problem to be clarified is the nature of the electronic state under the strong electron correlation and weak hybridization.

It is widely accepted that the simplest Hamiltonian to study the heavy fermion physics is the periodic Anderson model (PAM):

$$H=\sum_{k\sigma}\epsilon_k c^{\dagger}_{k\sigma}c_{k\sigma}+\epsilon_f\sum_{j\sigma}n^f_{j\sigma}+U_f\sum_j n^f_{j\uparrow}n^f_{j\downarrow}$$

$$+\frac{1}{\sqrt{L}}\sum_{jk\sigma}(V_k e^{ik\cdot r_j}c^{\dagger}_{k\sigma}f_{j\sigma}+\text{h.c})\,, \tag{1·1}$$

where $n^f_{j\sigma}=f^{\dagger}_{j\sigma}f_{j\sigma}$ and L is the total number of sites. The four terms describe a nondegenerate conduction band, f-electron level, the Coulomb repulsion on the f-orbital and the mixing between the conduction electron and f wave functions, respectively.

In the limit of nearly integral valence $n_f\to 1$, which is realized under the condition of a deep ϵ_f, a large U_f and a small V_k, the PAM can be replaced by the Kondo lattice

*) Dedicated to Professor J. Kanamori on the occasion of his sixtieth birthday.

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model (KLM) with the antiferromagnetic exchange coupling J:

$$H=\sum_{k\sigma}\epsilon_k c^{\dagger}_{k\sigma}c_{k\sigma}+\frac{J}{2}\sum_j \boldsymbol{S}_j\cdot c^{\dagger}_{j\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}c_{j\sigma'}\,, \tag{1·2}$$

where the magnitude of $\boldsymbol{S}_j$ is equal to 1/2 and the $\boldsymbol{\sigma}'$ are Pauli matrices. $c_{j\sigma}=L^{-1/2}\sum_k e^{ik\cdot r_j}c_{k\sigma}$ is the annihilation operator of the conduction-electron at the j-th site. The KLM should also be an appropriate Hamiltonian for low-energy physics. As shown in the Appendix, the PAM (1·1) generally produces in its effective Hamiltonian the second-order shift in energy and some additional intersite terms. However for the sake of simplicity we ignore those terms in this paper and concentrate ourselves to (1·2). The role of the second-order energy shift will be discussed in § 5.

The purpose of this paper is threefold. First, we wish to show explicitly with a simple variational approach that the spin-compensated Fermi-liquid state, in which the localized f-spins are compensated collectively with overlapping conduction-electron clouds, leads to a "large" Fermi surface. This problem is naturally related to the question of the saturation of the spin-compensation, which was raised by Nozieres.[4] Second, we wish to examine the nature of the spin-compensated state by using the variational Monte Carlo (VMC) method. In a previous paper[5] we applied the Gutzwiller approximation, which will be reexamined in this paper by comparing with the VMC results. Third, we wish to discuss the reason why the commonly used variational theory for the PAM is unstable against the ferromagnetic state, relating to it the present theory on the KLM.

This paper is organized as follows. Some forms of variational wave functions are proposed and examined in the next section. Then, the Gutzwiller approximation which was applied in Ref. 5) is briefly reviewed in § 3. In § 4 the nature of the spin-compensated Fermi-liquid state is studied with the VMC method and compared with the Gutzwiller approximation. Supplementary discussions are given in the last section.

§ 2. Variational wave functions

The most natural way of constructing a variational wave function for the KLM is to follow the singlet wave function for the ground state of the single-ion Kondo problem[6] and form a singlet cloud around each f-spin. The form of those overlapping clouds is then optimized variationally by properly taking into account the nonorthogonality of the clouds.

For N (total number of conduction electrons) $\leq L$ the simplest trial wave function would be

$$|\Psi\rangle=\prod_k^{(L-N)/2} c_{k\uparrow}c_{k\downarrow}\prod_l^{L}[f^{\dagger}_{l\uparrow}\tilde{c}^{\dagger}_{l\downarrow}-f^{\dagger}_{l\downarrow}\tilde{c}^{\dagger}_{l\uparrow}]|0\rangle\,, \tag{2·1}$$

where $\tilde{c}_{l\sigma}=L^{-1/2}\sum_k e^{ik\cdot r_l}a(k)c_{k\sigma}$ with the form factor $a(k)$ of the singlet cloud. $|0\rangle$ represents the vacuum. In (2·1) a singlet cloud is formed at each site and then $L-N$ excess electrons are taken away from the top of the conduction band. Notice that the local constraint that each site must be singly occupied by one f-electron is satisfied in

(2·1). $a(k)$ should be determined variationally. We note at this point that the singlet clouds are not orthogonal, i.e.,

$$[\tilde{c}_{j\sigma},\ \tilde{c}^{\dagger}_{l\sigma}]_{+}=L^{-1}\cdot\sum_{k}|a(k)|^{2}e^{ik\cdot(r_j-r_l)}\,,$$

which is generally nonzero for $j\neq l$.

The wave function can be written into another form by introducing explicitly a projection operator $\hat{P}$ onto the subspace in which each site is always occupied one f-electron:

$$\hat{P}=\prod_{j}[n^{f}_{j\uparrow}(1-n^{f}_{j\downarrow})+n^{f}_{j\downarrow}(1-n^{f}_{j\uparrow})]\,. \tag{2·2}$$

In fact it is easy to observe that

$$\prod_{l}^{L}[f^{\dagger}_{l\uparrow}\,\tilde{c}^{\dagger}_{l\downarrow}-f^{\dagger}_{l\downarrow}\,\tilde{c}^{\dagger}_{l\uparrow}]|0\rangle=\prod_{l}^{L}[\,\tilde{c}^{\dagger}_{l\uparrow}f_{l\uparrow}+\tilde{c}^{\dagger}_{l\downarrow}f_{l\downarrow}]\prod_{m}^{L}f^{\dagger}_{m\uparrow}f^{\dagger}_{m\downarrow}|0\rangle$$

$$=\lambda^{-L}\hat{P}\prod_{\sigma}\prod_{l}^{L}(\lambda+\tilde{c}^{\dagger}_{l\sigma}f_{l\sigma})\prod_{m}^{L}f^{\dagger}_{m\uparrow}f^{\dagger}_{m\downarrow}|0\rangle \tag{2·3}$$

holds. λ is an arbitrary number because of the presence of $\hat{P}$. Now we use operators in k-space to rewrite (2·3) further. Then (2·3) is reduced to $\lambda^{-L}\hat{P}\prod_{k\sigma}(\lambda f^{\dagger}_{k\sigma}+a(k)^{*}c^{\dagger}_{k\sigma})|0\rangle$. Here $f^{\dagger}_{k\sigma}$ is the Fourier transform of $f^{\dagger}_{l\sigma}$. Substituting this into (2·1), we find finally

$$|\Psi\rangle=\hat{P}\prod_{\sigma}\prod_{k}^{(N+L)/2}[\lambda f^{\dagger}_{k\sigma}+a(k)^{*}c^{\dagger}_{k\sigma}]|0\rangle\,, \tag{2·4}$$

where the product in k is taken over the lowest $(N+L)/2$ states. A constant factor irrelevant to calculating expectation values has been dropped in (2·4). Thus we have shown that (2·1) is equivalent to (2·4), which is in essence a *Gutzwiller-projected mixed-band* wave function.

Instead of (2·1) one could start from a different form, in which first $N+L$ electrons fill the conduction band from the bottom and then a hole is trapped around each f-spin to form a singlet:

$$|\Psi\rangle=\prod_{l}^{L}[f^{\dagger}_{l\uparrow}\,\tilde{c}_{l\uparrow}+f^{\dagger}_{l\downarrow}\,\tilde{c}_{l\downarrow}]\prod_{k}^{(L+N)/2}c^{\dagger}_{k\uparrow}c^{\dagger}_{k\downarrow}|0\rangle\,. \tag{2·5}$$

Here again the form factor of the hole is introduced as $\tilde{c}_{l\sigma}=L^{-1/2}\sum_{k}e^{ik\cdot r_l}a(k)c_{k\sigma}$. Actually (2·5) is the same wave function as we studied in our previous paper.[5] A procedure, which led us from (2·1) to (2·4), allows us to rewrite (2·5). In fact, noting that

$$\prod_{l}^{L}[f^{\dagger}_{l\uparrow}\,\tilde{c}_{l\uparrow}+f^{\dagger}_{l\downarrow}\,\tilde{c}_{l\downarrow}]=\lambda^{-L}\hat{P}\prod_{\sigma}\prod_{l}^{L}[\lambda+f^{\dagger}_{l\sigma}\,\tilde{c}_{l\sigma}]$$

$$=\lambda^{-L}\hat{P}\prod_{\sigma}\prod_{k}[\lambda+a(k)f^{\dagger}_{k\sigma}c_{k\sigma}] \tag{2·6}$$

holds, (2·5) can be rewritten as

$$|\Psi\rangle=\hat{P}\prod_{\sigma}\prod_{k}^{(N+L)/2}[\lambda c_{k\sigma}^{\dagger}+a(k)f_{k\sigma}^{\dagger}]|0\rangle\,, \tag{2·7}$$

which is exactly the same as (2·4), if a replacement $a(k)\to[a(k)^*]^{-1}$ is made. A constant factor irrelevant to later discussions has been taken off in (2·7). Since the optimum form of $a(k)$ is determined variationally in both cases, (2·4) and (2·7) are equivalent.

An important point is that our variational wave function ((2·4) or (2·7)) is essentially a Gutzwiller-projected mixed-band wave function, in which the lower mixed-band is filled up to $(N+L)/2$. The local constraint shows up only in the form of $\hat{P}$. Let us recall in this connection that a similar wave function has been used in the variational theory for the $U_f\to\infty$ PAM.[7] In the latter case $\hat{P}$ is defined as $\hat{P}=\prod_l[1-n_{l\uparrow}^f n_{l\downarrow}^f]$, where only the doubly occupied states of f-electrons are projected out.

Let us turn to the case $N\geq L$. An analogy to $N\leq L$ suggests us to construct a variational wave function for this case as

$$|\Psi\rangle=\prod_{k}^{(N-L)/2}c_{k\uparrow}^{\dagger}c_{k\downarrow}^{\dagger}\prod_{l}^{L}[f_{l\uparrow}^{\dagger}\tilde{c}_{l\downarrow}^{\dagger}-f_{l\downarrow}^{\dagger}\tilde{c}_{l\uparrow}^{\dagger}]|0\rangle\,. \tag{2·8}$$

An introduction of $\hat{P}$ enables us to express (2·8) in a form similar to (2·4)

$$|\Psi\rangle=\hat{P}\prod_{\sigma}\prod_{k}^{(N-L)/2}[-a(k)^*f_{k\sigma}^{\dagger}+\lambda c_{k\sigma}^{\dagger}]\cdot\prod_{k'}[\lambda f_{k'\sigma}^{\dagger}+a(k')^*c_{k'\sigma}^{\dagger}]|0\rangle\,. \tag{2·9}$$

The factor $\prod_l^L[f_{l\uparrow}^{\dagger}\tilde{c}_{l\downarrow}^{\dagger}-f_{l\downarrow}^{\dagger}\tilde{c}_{l\uparrow}^{\dagger}]$ in (2·8) has been transformed into the filled lower mixed-band $\prod_{k'}[\lambda f_{k'\sigma}^{\dagger}+a(k')^*c_{k'\sigma}^{\dagger}]$, while the extra $N-L$ electrons $\prod_k^{(N-L)/2}c_{k\uparrow}^{\dagger}c_{k\downarrow}^{\dagger}$ go into the bottom of the upper-mixed band as $\prod_\sigma\prod_k^{(N-L)/2}[-a(k)^*f_{k\sigma}^{\dagger}+\lambda c_{k\sigma}^{\dagger}]$.

The representation in terms of the Gutzwiller-projected mixed-band is useful in many respects. First, it shows clearly that the number of (localized) f-electrons appears in the size of Fermi surface in accordance with Luttinger sum rule. Second, the spin-compensation occurs collectively, although we started from a superposition of local Kondo singlets. This is due to the fermionic nature of Kondo clouds. Third, it provides us with a link to the variational theory for the PAM. The last point will be discussed further in § 5.

In the following sections we focus our discussions on the case $N\leq L$, for which (2·5) (or equivalently (2·7)) is used as a variational wave function.

§ 3. Gutzwiller approximation

The next task is to evaluate the average of H for our variational wave function (2·5) (or (2·7)):

$$\langle H\rangle=\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}\,. \tag{3·1}$$

Actually this was already carried out in a previous paper within the Gutzwiller approximation.[5] Here we summarize the main results of Ref. 5) without going into mathematical details. In contrast to Ref. 5) we present rather a complementary

intuitive derivation.

Briefly speaking, the Gutzwiller approximation[11),12),15)~17)] is a statistical treatment of the average, in which the local constraint for each site to be occupied always by one f-electron is relaxed and is satisfied only in a statistical sense. For convenience we include explicitly the f-electron energy $\epsilon_f \sum_{j\sigma} n_{j\sigma}^f$ in (2·1).

The mixed-band representation of the wave function (2·7) is useful to understand the essence of the Gutzwiller approximation. First, the mixed-band form immediately suggests that the portion of conduction-electron part and f-electron part in the ground state should be

$$\langle c_{k\sigma}^{\dagger} c_{k\sigma} \rangle = \frac{\lambda^2}{\lambda^2 + a(k)^2}, \tag{3·2}$$

$$\langle f_{j\sigma}^{\dagger} f_{j\sigma} \rangle = \frac{1}{L} \sum_k \frac{a(k)^2}{\lambda^2 + a(k)^2}, \tag{3·3}$$

in the Gutzwiller approximation. The arbitrary parameter λ, which is the same as $e^{-\mu/2}$ in our previous paper,[5)] is fixed so as to fulfill the requirement

$$1 = \sum_{\sigma} \langle f_{j\sigma}^{\dagger} f_{j\sigma} \rangle = \frac{2}{L} \sum_k \frac{a(k)^2}{\lambda^2 + a(k)^2}. \tag{3·4}$$

Having (3·2) and (3·3), we obtain the sum of one-electron energies as

$$\langle \sum_{k\sigma} \epsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + \epsilon_f \sum_{j\sigma} n_{j\sigma}^f \rangle = 2 \sum_k \frac{(\epsilon_f - \epsilon_k) a^2(k)}{\lambda^2 + a^2(k)}, \tag{3·5}$$

where $\sum_k \epsilon_k = 0$ is used to define the origin of our energy scale.

As for the exchange energy we take up a transverse term in (1·2)

$$\langle S_j^{+} c_{j\downarrow}^{\dagger} c_{j\uparrow} \rangle = \langle f_{j\uparrow}^{\dagger} f_{j\downarrow} c_{j\downarrow}^{\dagger} c_{j\uparrow} \rangle = - \langle f_{j\uparrow}^{\dagger} c_{j\uparrow} c_{j\downarrow}^{\dagger} f_{j\downarrow} \rangle . \tag{3·6}$$

This quantity can be replaced, within the Gutzwiller approximation, by a product of two *independent* averages for $\uparrow$ and $\downarrow$ spins over the *unprojected* mixed-band, which has to be however multiplied by a correction factor 2 due to the local constraint:

$$-2 \left[\frac{1}{L} \sum_k \frac{\lambda a(k)}{\lambda^2 + a(k)^2} \right]^2 . \tag{3·7}$$

The reason for the factor 2 is the following.[18)] In the unprojected wave function there are 4 possibilities for the f-electron at each site: vacant state, $\uparrow$-spin, $\downarrow$-spin and double occupancy, among which vacant and doubly occupied states are nonmagnetic so that they do not contribute to the exchange energy. On the other hand, singly occupied $\uparrow$- and $\downarrow$-states survive after an application of the projection operator $\hat{P}$. Therefore the factor 2 is needed in order to take into account $\hat{P}$ in a statistical way.[18)]

Using (3·7) and the isotropy of the exchange interaction, we obtain for the average of the exchange energy

$$\frac{J}{2} \sum_{\sigma\sigma'} \langle \boldsymbol{S}_j \cdot c_{j\sigma}^{\dagger} \boldsymbol{\sigma}_{\sigma\sigma'} c_{j\sigma'} \rangle = -3J \cdot \left[\frac{1}{L} \sum_k \frac{\lambda a(k)}{\lambda^2 + a(k)^2} \right]^2 . \tag{3·8}$$

The complete expression for the total energy is then

$$\frac{\langle H\rangle}{L}=\frac{2}{L}\cdot\sum_k u(k)[\epsilon_f-\epsilon_k]-3J\cdot\left[\frac{1}{L}\sum_k\sqrt{u(k)[1-u(k)]}\right]^2, \tag{3·9}$$

where $u(k)=a(k)^2/[\lambda^2+a(k)^2]$ and the constraint (3·4) is to be satisfied.

The optimum from of $a(k)$ can be determined by imposing, together with (3·4), $\partial\langle H\rangle/\partial a(k)=0$. The result is[5]

$$a(k)=\frac{\alpha\lambda^2}{\tilde{\epsilon}_f-\epsilon_k+\sqrt{(\tilde{\epsilon}_f-\epsilon_k)^2+(\alpha\lambda)^2}}, \tag{3·10}$$

where

$$\alpha=3J\frac{1}{L}\sum_k\frac{a(k)}{\lambda^2+a(k)^2}, \tag{3·11}$$

$$\tilde{\epsilon}_f=\epsilon_f-\frac{1}{AL}\sum_k\frac{\left[\epsilon_f-\epsilon_k+\frac{\alpha}{2}a(k)\right]a(k)^2-\frac{\alpha}{2}a(k)\lambda^2}{[\lambda^2+a(k)^2]^2}, \tag{3·12}$$

$$A=\frac{1}{L}\sum_k\frac{a(k)^2}{[\lambda^2+a(k)^2]^2}. \tag{3·13}$$

The form (3·10) is essentially what one expects from an "effective hybridization Ansatz", in which $\tilde{\epsilon}_f$ is the "effective f-level" and $\alpha\lambda$ is the "effective hybridization". We will not go further into the consequences of the Gutzwiller approximation here, since it was described in details in Ref. 5) and we shall come back to this problem in the next section.

§ 4. A variational Monte Carlo study

The Gutzwiller approximation is based on a statistical treatment to quantum mechanical matrix elements, which definitely needs a check by a different method. For this reason we now apply the variational Monte Carlo (VMC) method[9),19)] to the trial wave function (2·7).

The VMC method[20),21)] is an approach of evaluating directly quantum mechanical averages by the Monte Carlo procedure without introducing uncontrolled approximations, which may violate the variational principle. The VMC method is particularly suited for taking into account the local constraint of our problem that the number of f-electrons at each site should be strictly 1. This is an evident merit of this approach over other theories and is in contrast to the Gutzwiller approximation.

Since the analysis of $a(k)$ in § 3 led to the form of (3·10), we employ it and take $\tilde{\epsilon}_f$ and $\tilde{V}=\alpha\lambda/2$ as variational parameters:

$$a(k)=\frac{2\tilde{V}}{\tilde{\epsilon}_f-\epsilon_k+\sqrt{(\tilde{\epsilon}_f-\epsilon_k)^2+4\tilde{V}^2}}. \tag{4·1}$$

The additional factor λ in the nominator of (3·10) is omitted, since it is irrelevant as far as we work always in the subspace where each site is occupied by *one* f-electron. In fact, within this subspace λ is an arbitrary constant, as the derivation of (2·7)

showed. We note again that (4·1) is the same form as that appearing in a similar variational study of the PAM.[9]

Although the formulation and the method are general, we restrict our applications to a one-dimensional model for simplicity: $\epsilon_k=-2t\cos(k)$. Actually the variational Monte Carlo method for the present case is similar to that for the PAM, since the wave function (2·7) has a form of mixed-bands. The only difference lies in the projection operator $\hat{P}=\Pi_j[n_{j\uparrow}^f(1-n_{j\downarrow}^f)+n_{j\downarrow}^f(1-n_{j\uparrow}^f)]$. The commonly used variational wave function for the $U_f\to\infty$ PAM[7)~12)] has the same form as (2·7), but $\hat{P}$ is replaced by $\Pi_j[1-n_{j\uparrow}^f n_{j\downarrow}^f]$. Therefore the VMC method, which was used previously for the PAM, can be easily extended to the KLM. In the present work the configuration is changed in two types of trials: One is a move of a randomly chosen conduction-electron to one of the neighboring sites and the other is a simultaneous spin-flip of an f-electron and a conduction-electron on the same site. These trials are

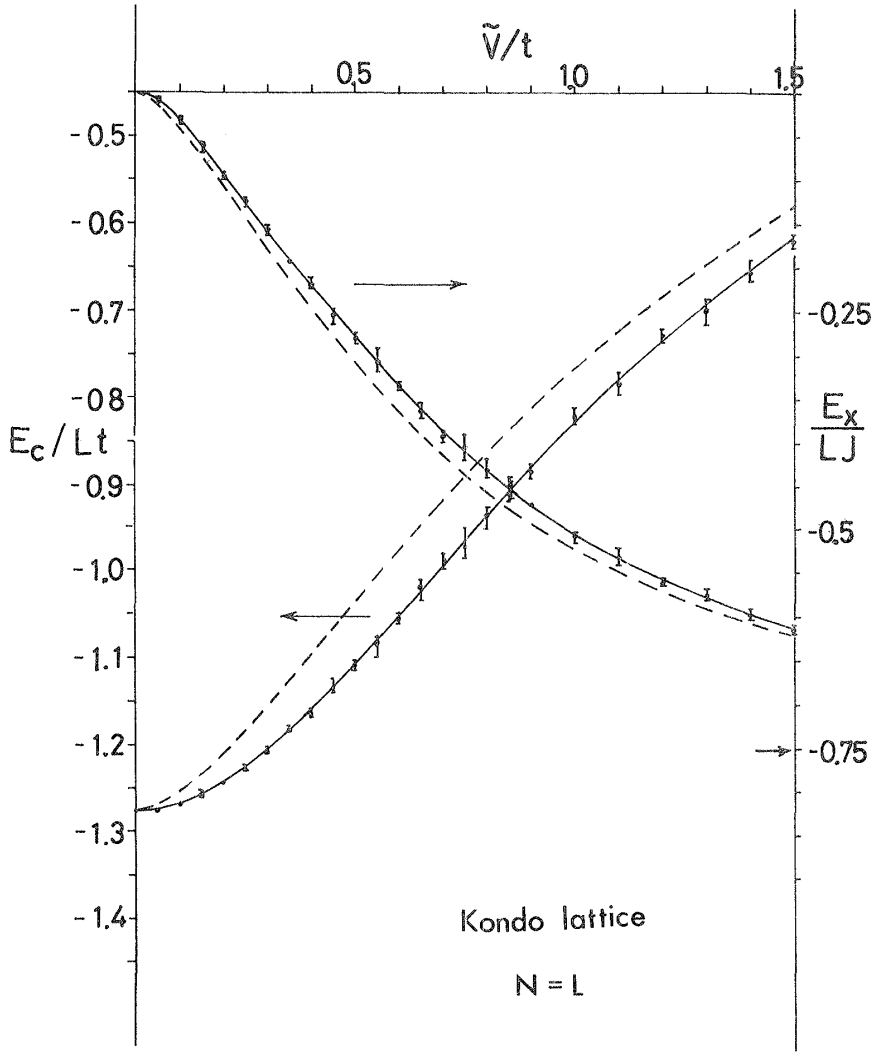

Fig. 1. The conduction-band energy per site E_c/tL and the exchange energy per site E_x/JL for the semiconducting case $n=N/L=1$. $\tilde{\epsilon}_f$ is chosen to be 0. The Monte Carlo calculation was carried out on $N=L=30$. An average over 5000 MC steps is plotted; by dividing into 5 1000-MCS samples the maximum and minimum are shown with error bars. The arrow on the right vertical axis indicates the value of E_x/tL for $\tilde{V}/t\to\infty$. The results of the Gutzwiller approximation, (4·2) and (4·3), are shown with the broken lines.

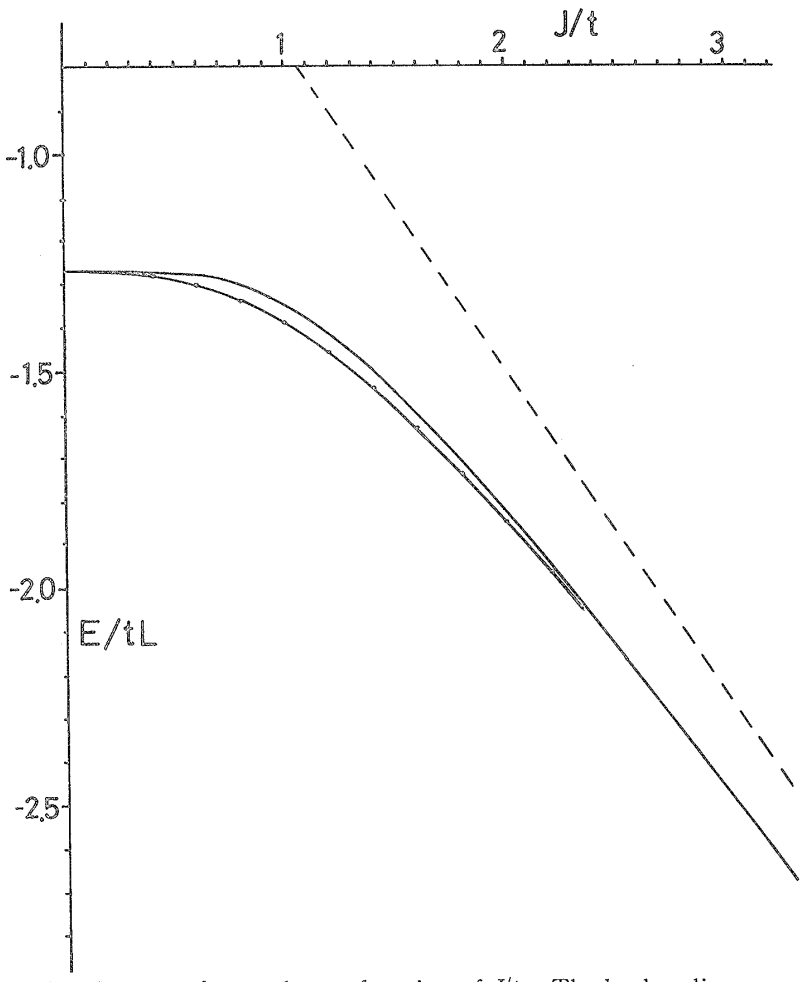

Fig. 2. The variational energy for $n=1$ as a function of J/t. The broken line represents the energy for the collection of local singlets. The solid line connecting solid circles represents the VMC result, while the Gutzwiller approximation is shown with the solid line.

either accepted as a new configuration or rejected according to the standard Monte Carlo procedure.[20),21)]

Let us start from examining the semiconducting case with $N=L$. For this case $\tilde{\epsilon}_f$ in (4·1) can be fixed at the band center, $\tilde{\epsilon}_f=0$, because of the electron-hole symmetry; therefore $\tilde{V}$ is the sole variational parameter that controls the form factor of the Kondo cloud. Figure 1 shows the average of the conduction-band and exchange energies in (1·2), which was carried out over the variational wave function (2·7). In addition to $N=L=30$ presented in Fig. 1, we have examined a larger system with $N=L=58$ to check the size dependence; within the statistical accuracy no significant difference has been found between the two cases. The decoupling of conduction electron and f bands, i.e., $\tilde{V}\to 0$, is the most favorable for the conduction-band energy. On the other hand a larger $\tilde{V}$ leads to a more localized Kondo cloud, for which the exchange energy is gained more effectively. The balance of these two energies determines the minimum of the variational energy E_g as a function of J/t, which is presented in Fig. 2.

It is interesting to compare the VMC results with the Gutzwiller approximation. For the latter case one can analytically evaluate the average of the conduction-band and exchange energies in (3·9), taking the one-dimensional model $\epsilon_k=-2t\cos k$. The

result is as follows:

$$\frac{\langle H_c\rangle}{tL}=-\frac{4}{\pi}\left[\sqrt{1+(\tilde{V}/t)^2}E(k)-\frac{(\tilde{V}/t)^2}{\sqrt{1+(\tilde{V}/t)^2}}K(k)\right], \tag{4·2}$$

$$\frac{\langle H_x\rangle}{JL}=-3\left[\frac{\tilde{V}/t}{\sqrt{1+(\tilde{V}/t)^2}}\frac{1}{\pi}K(k)\right]^2, \tag{4·3}$$

where $K(k)$ and $E(k)$ are the complete elliptic integral of the first and second kinds, respectively and $k=1/\sqrt{1+(\tilde{V}/t)^2}$ is the modulus. Those expressions of the Gutzwiller approximation are compared in Fig. 1 with the VMC results, which are supposed to be exact within the variational wave function and the statistical errors. Incidentally (4·2) and (4·3) give the minimum of the total energy with respect to $\tilde{V}/t$ at

$$\frac{J}{t}=\frac{2\pi}{3}\frac{1}{kK(k)}, \tag{4·4}$$

which reduces to $\tilde{V}/t=\sqrt{2}e^{-2\pi t/3J}$ for the weak coupling limit.

It is clear from Fig. 1 that the Gutzwiller approximation overestimates the exchange energy and underestimates the conduction-band energy. Because of an approximate cancellation between the two the resulting total energy shown in Fig. 2 is not so much different from the VMC result. Let us remember that we took a one-dimensional model for simplicity. According to our experience on the Hubbard model[19),22),23)] the difference between the Gutzwiller approximation and the VMC is the largest in one dimension and diminishes rapidly as the dimension increases. We expect it to be true also in the KLM.

Let us turn to a metallic case. The VMC calculation has been extended by taking $n=N/L=3/4$ as a typical case. In this case we have 2 variational parameters $\tilde{\epsilon}_f$ and $\tilde{V}$. Instead of a complete search for the energy minimum with respect to 2 parameters, we are rather guided by the the Gutzwiller approximation[5)] showing that for the weak coupling regime the optimal $\tilde{\epsilon}_f$ does not deviate so much from the value, for which the mixed-band can accomodate exactly one f-electron per site in the limit of $\tilde{V}\to 0$. Therefore we fix $\tilde{\epsilon}_f$ at this value for simplicity, leaving more complete analysis for a future study. The results for the conduction-electron energy and exchange energy, which correspond to Fig. 1, are shown in Fig. 3. An evident feature of Fig. 3 is that E_x/JL is reduced compared with Fig. 1 because of less conduction electrons per spin available for the compensation. Otherwise the results are similar to the previous one for $n=1$.

We now look into some physical quantities of interest. In connection with the concept of heavy fermions the momentum distribution function $n(k)$ is the most important quantity. Figure 4 shows $n(k)$ for $n=3/4$, which is chosen as a typical metallic case. As already pointed out in Ref. 5), the two major features of interest are the jump at the "large" Fermi surface and a gradual change around the "small" Fermi surface. This feature of $n(k)$ can be interpreted as follows. The mixed-band form of the wave function tells us that the states below the "small" Fermi surface are conduction-electron-like, while the states between the "large" and "small" Fermi

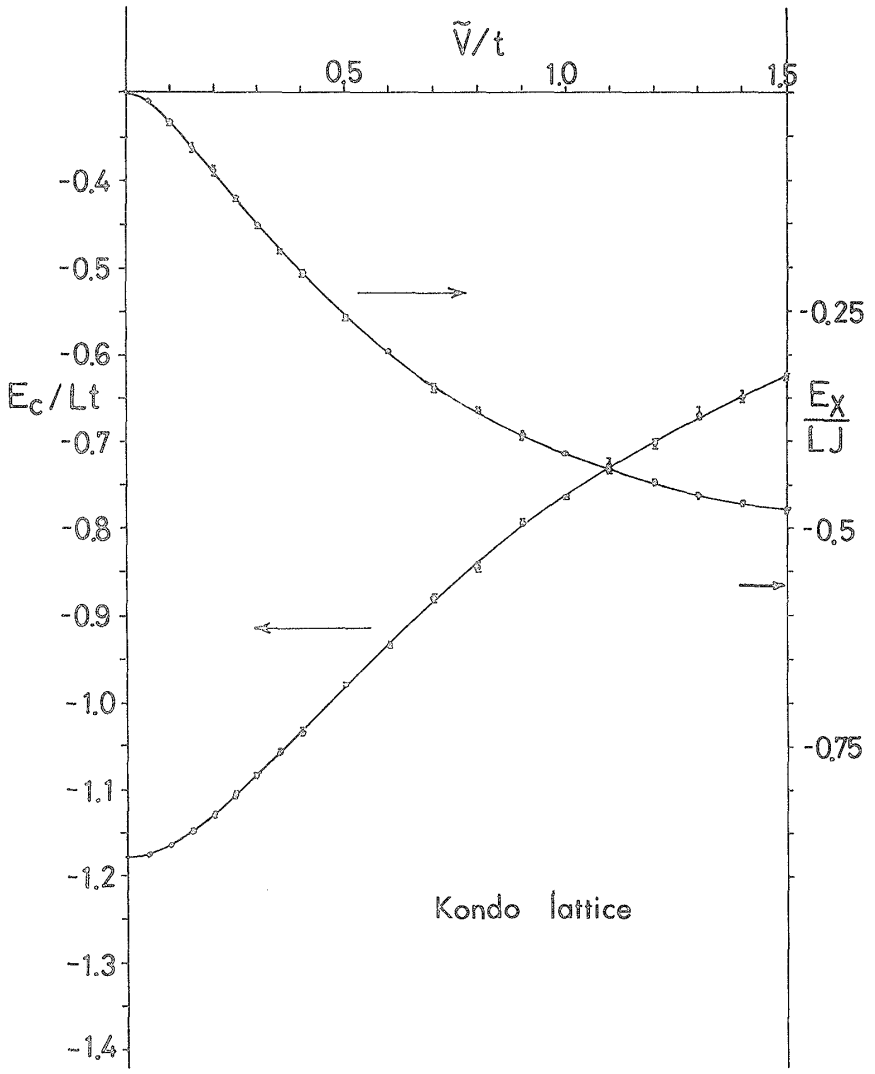

Fig. 3. The conduction-band energy per site E_c/tL and the exchange energy per site E_x/JL for a metallic case $n=N/L=3/4$. $\tilde{\epsilon}_f/t$ is taken as -0.7630. The Monte Carlo calculation was carried out on $N=30$ and $L=40$. An average over 5000 MC steps is plotted; by dividing into 5 1000-MCS samples the maximum and minimum are shown with error bars. The arrow on the right vertical axis indicates the value of E_x/tL for $\tilde{V}/t\to\infty$.

surfaces are mainly f-like. The jump at k_F is small, suggesting that conduction electrons are strongly correlated and heavy. The vanishing contribution to $n(k)$ above k_F is a direct consequence of the approximate nature of the variational wave function (2·7) so that it should not be taken seriously. Needless to say, $n(k)$ does not show any jump in the semiconducting case with $n=1$.

We now turn to intersite spin correlations $\langle S_{j\mu}\cdot S_{l\nu}\rangle$ and their Fourier transforms:

$$S_{\mu\nu}(q)=\frac{1}{L}\sum_{j,l}4\langle S^z_{j\mu}\cdot S^z_{l\nu}\rangle e^{iq\cdot(r_j-r_l)}, \tag{4·5}$$

where μ and ν represent either c or f. The isotropy of the spin correlation, i.e., $\langle S^+_{j\mu}\cdot S^-_{l\nu}\rangle=2\langle S^z_{j\mu}\cdot S^z_{l\nu}\rangle$, is satisfied statistically in the VMC method. This was used to check the reliability of our Monte Carlo calculation.

An example of $S_{\mu\nu}(q)$ for $n=1$ and $3/4$ is presented in Fig. 5. In the case $n=1$ the

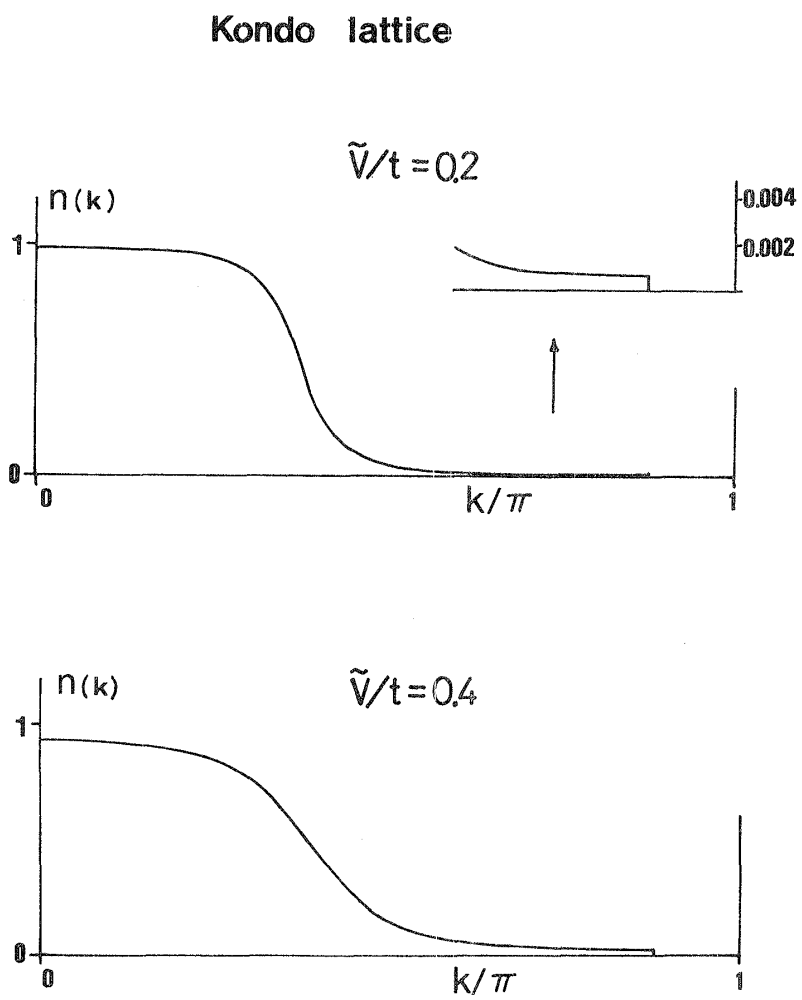

Fig. 4. The momentum distribution function $n(k)$ for $n=3/4$. Two cases corresponding to $\tilde{V}/t=0.2$ and 0.4 are shown; $\tilde{\epsilon}_f/t$ is fixed at -0.7630, as described in the text.

f-f spin correlation is antiferromagnetic and much enhanced. The f-c correlation is antiferromagnetic as expected. On the other hand, the spin correlation is different in $n=3/4$, where the f-f spin correlation is enhanced, but a dominant peak of $S(k)$ is shifted to an incommensurate position. These results remind us of similar ones in the PAM.[9] As described there, this behavior of $S(k)$ can be interpreted as due to the mixed-band wave function rather than RKKY-type magnetic coupling, which is not taken into account in our wave function. The latter effect is expected to be important.

§ 5. Summary and discussion

As a continuation to Ref. 5) the simplest variational wave function has been constructed and studied for the spin-compensated Fermi-liquid ground state in the Kondo lattice. Although we started from a superposition of local Kondo singlets, it has turned out to be equivalent to a picture that the localized f-spins are compensated collectively with overlapping conduction-electron clouds. This is due to the fermionic nature of Kondo clouds. It is shown explicitly that this compensation results in forming a "large" Fermi surface, in which the number of f-electrons takes part. In

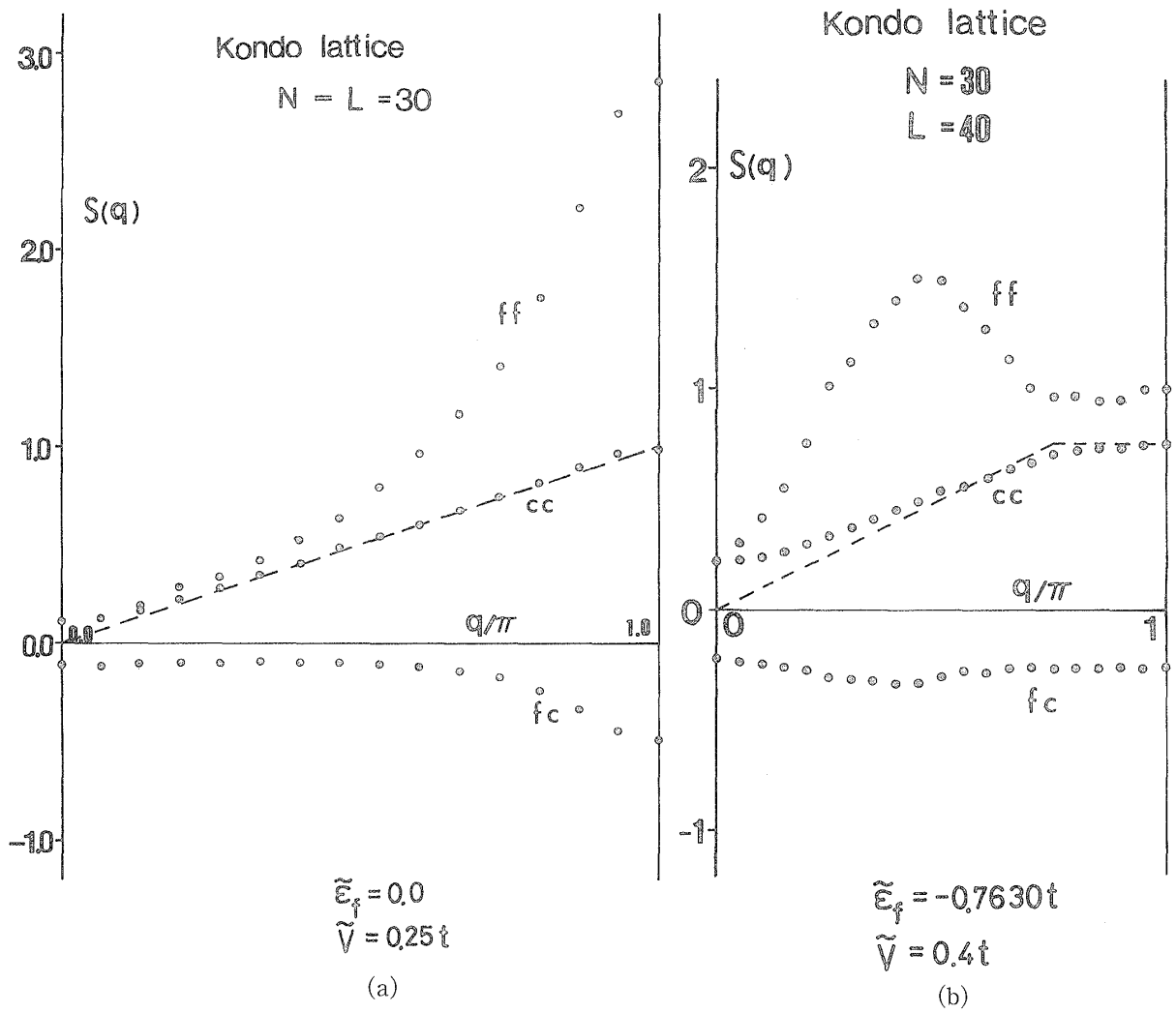

Fig. 5. The f-f, f-c, c-c spin correlation functions for (a) n=1 and (b) n=3/4. The broken line shows the spin correlation for noninteracting electrons.

other words the f-electrons participate in the "Fermi surface" notwithstanding their complete localization in the Kondo Hamiltonian. This is a result of the phase shift of conduction electrons caused by localized spins. The nature of this ground state has been examined with the Gutzwiller approximation and the variational Monte Carlo (VMC) method. The results show that heavy electrons are formed as a consequencce of overlapping singlet clouds.

Let us discuss the relation between the variational theory for the KLM and that for the PAM . As already pointed out in § 2, our variational wave function has a close similarity, in its form, to the commonly used variational wave function for the PAM. Notice that the KLM with the antiferromagnetic exchange coupling H_{KLM} is an effective Hamiltonian, which can be derived from the PAM H_{PAM} by the Schrieffer-Wolff transformation:[14]

$$H_{\mathrm{KLM}}=e^{iS}H_{\mathrm{PAM}}e^{-iS}\,, \tag{5·1}$$

$$\Psi_{\mathrm{KLM}}=e^{iS}\Psi_{\mathrm{PAM}}\,. \tag{5·2}$$

(See the Appendix.) Therefore our variational wave function for the KLM Ψ_{KLM} amounts to taking into account virtual processes by the factor e^{-iS} in $\Psi_{\mathrm{PAM}}=e^{-iS}\Psi_{\mathrm{KLM}}$. For this reason our variational theory on the KLM should be a better description than the similar variational theory on the PAM.

Our first argument is based on energetics. It is well known that in the variational theory the (collective singlet) Fermi liquid state of the PAM is unstable against a ferromagnetic ordering of the f-spins.[24] This is mainly due to the lack of a second-order term in the ground state energy of the Fermi liquid state, since the energy of the ferromagnetic state contains such an energy lowering. This weak point is remedied in our variational theory for the KLM: The second-order shift is generated by the Schrieffer-Wolff transformation as a constant term which is independent of the configuration of the f-spins, and is therefore usually omitted when writing down the KLM Hamiltonian. It should be, however, taken into account when we use our formalism to make a statement about the ground state energy of the Kondo limit of the PAM: From (A·5) for $U_f\to\infty$ the full expression is

$$H_{\mathrm{PAM}}\Longrightarrow H_{\mathrm{KLM}}+L\epsilon_f-\sum_{k}^{\epsilon_k>\tilde{\epsilon}_f{}^0}\frac{|V_k|^2}{\epsilon_k-\epsilon_f}\,, \tag{5·3}$$

where $\tilde{\epsilon}_f{}^0$ is the $V_k=0$ value of the effective f-level (or, equivalently, the Fermi-energy corresponding to the small Fermi surface). For a band $0\le\epsilon_k\le W$ with a constant density of states, and assuming a constant hybridization $V_k\equiv V$, the singlet ground state energy is obtained as

$$\frac{1}{L}\langle H_{\mathrm{PAM}}\rangle_V=\frac{1}{L}\langle H_{\mathrm{PAM}}\rangle_{V=0}-\frac{V^2}{W}\ln\frac{W-\epsilon_f}{\tilde{\epsilon}_f{}^0-\epsilon_f}+\frac{1}{L}(\langle H_{\mathrm{KLM}}\rangle_J-\langle H_{\mathrm{KLM}}\rangle_{J=0})\,, \tag{5·4}$$

where J is the KLM exchange coupling identified from (A·5). The second-order term is the same as that obtained in Ref. 24) for a simple ferromagnetic trial state for the PAM; the present treatment makes it clear that the same energy lowering has to result for any arrangement of the f-spins and taken in itself, it does not signal a magnetic instability. In fact, the last term in (5·4) describes the additional Kondo binding which acts to stabilize a Fermi-liquid-type state. We are, of course, not claiming that magnetic ordering is thereby excluded; only that an eventual magnetic instability has to arise from terms higher order in V (presumably $\propto V^4/W^3$). This conclusion is well known in the Kondo lattice literature, but it is less self-evident in the variational description where one has to keep track also of energy shifts which are common to all (or at least a large class of) configurations, and have thus "no direct physical meaning". Our considerations were formulated for the extremely asymmetric Anderson model but it is clear that similar results should be obtained in the large-U_f-limit of the symmetrical PAM. On the basis of numerical simulations, Blankenbecler et al.[25] noticed that for large U_f, the dominating contribution to the ground state energy is second-order in V; our reasoning indicates that this need not be associated with the breakdown of the Fermi-liquid (or effective hybridized band) picture.

We can also point out the general similarity to the case of the Hubbard model: As it was pointed out by Gros, Joynt and Rice,[26] a variational theory for the effective

Hamiltonian in the strong-coupling limit is superior to a similar variational theory for the original Hubbard model since in the former, certain virtual processes are taken into account through the canonical transformation.

Although there are several nice and encouraging features in our variational theory, we have to remember at the same time that the proposed wave function is based on a natural extension of the *lowest-order* Yosida's singlet wave function[6] to the Kondo lattice and is just the "first-order" approximation. Therefore improvements of the wave function are needed. However we believe the "large" Fermi surface, which shows up already in our simplest wave function, should remain as long as the ground state is a Fermi liquid. What has to be supplemented to the wave function in the next step is the intersite (antiferromagnetic) correlations, which are definitely important. In addition, we assumed the Fermi-liquid state for any electron density $n=N/L$ and have not examined other possibilities. For instance, some other state different from the Fermi-liquid state may be realized for a small n. Those interesting problems are left for a future study.

Finally, we wish to mention that as many researchers pointed out, the Kondo lattice Hamiltonian may be applicable also to the problem of high-T_c oxides. In fact our local Kondo singlet is similar to the Zhang-Rice singlet.[27] The present work demonstrates how a formation of the Fermi-liquid is possible from the Zhang-Rice singlets with a finite density. More work is needed to understand further the difference and similarity in the heavy fermion and high-T_c problems.

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Appendix

Let us apply the Schrieffer-Wolff transformation[14] to $H\Psi=E\Psi$:

$$e^{iS}He^{-iS}\cdot e^{iS}\Psi=Ee^{iS}\Psi\,, \tag{A·1}$$

in which S is chosen perturbatively so as to eliminate the off-diagonal term of the mixing in (1):

$$S=\frac{1}{\sqrt{L}}\sum_{jk\sigma}[(g_k^{(+)}e^{ik\cdot r_j}c_{k\sigma}^{\dagger}f_{j\sigma}n_{j-\sigma}^{f}+g_k^{(-)}e^{ik\cdot r_j}c_{k\sigma}^{\dagger}f_{j\sigma}(1-n_{j-\sigma}^{f}))+\text{h.c.}]\,. \tag{A·2}$$

$g_k^{(\pm)}$ are given, up to the first order of V_k, by $g_k^{(+)}=-iV_k/(\epsilon_k-\epsilon_f-U_f)$ and $g_k^{(-)}=-iV_k/(\epsilon_k-\epsilon_f)$, respectively. The resulting effective Hamiltonian $\tilde{H}\equiv e^{iS}He^{-iS}$ is then

$$\tilde{H}=H+[iS,H]+\frac{1}{2}[iS,[iS,H]]+\cdots$$
$$=\sum_{k\sigma}\epsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}+H_2+O(V^3), \tag{A·3}$$

where

$$H_2=\frac{1}{2L}\sum_{jkk'\sigma}\left[\frac{1}{\epsilon_k-\epsilon_f}-\frac{1}{\epsilon_k-\epsilon_f-U_f}\right]V_kV_{k'}^{*}e^{i(k-k')\cdot r_j}c_{k\sigma}^{\dagger}c_{-k'-\sigma}^{\dagger}f_{j-\sigma}f_{j\sigma}$$
$$+\frac{1}{2L}\sum_{ljk\sigma}\left[-\frac{|V_k|^2}{\epsilon_k-\epsilon_f}e^{ik\cdot(r_j-r_l)}f_{l\sigma}^{\dagger}f_{j\sigma}(1-n_{j-\sigma})\right.$$
$$\left.-\frac{|V_k|^2}{\epsilon_k-\epsilon_f-U_f}e^{ik\cdot(r_j-r_l)}f_{l\sigma}^{\dagger}f_{j\sigma}n_{j-\sigma}\right]$$
$$+\frac{1}{2L}\sum_{jkk'}V_kV_{k'}^{*}e^{i(k-k')\cdot r_j}$$
$$\times\left[\frac{1}{\epsilon_k-\epsilon_f}\left((c_k^{\dagger}\boldsymbol{S}c_{k'})\cdot(f_j^{\dagger}\boldsymbol{S}f_j)+\frac{1}{2}(c_k^{\dagger}c_{k'})\cdot(f_jf_j^{\dagger})\right)\right.$$
$$\left.-\frac{1}{\epsilon_k-\epsilon_f-U_f}\left((c_k^{\dagger}\boldsymbol{S}c_{k'})\cdot(f_j^{\dagger}\boldsymbol{S}f_j)-\frac{1}{2}(c_k^{\dagger}c_{k'})\cdot(f_j^{\dagger}f_j)\right)\right]+\text{h.c.}, \tag{A·4}$$

where $(c_k^{\dagger}\boldsymbol{S}c_{k'})\equiv\sum_{\sigma\sigma'}c_{k\sigma}^{\dagger}\boldsymbol{S}_{\sigma\sigma'}c_{k'\sigma'}$, $(f_j^{\dagger}\boldsymbol{S}f_j)\equiv\sum_{\sigma\sigma'}f_{j\sigma}^{\dagger}\boldsymbol{S}_{\sigma\sigma'}f_{j\sigma'}$, $(c_k^{\dagger}c_{k'})\equiv\sum_{\sigma}c_{k\sigma}^{\dagger}c_{k'\sigma}$, $(f_j^{\dagger}f_j)\equiv\sum_{\sigma}f_{j\sigma}^{\dagger}f_{j\sigma}$ and $(f_jf_j^{\dagger})\equiv\sum_{\sigma}f_{j\sigma}f_{j\sigma}^{\dagger}$. For $\epsilon_f\ll 0$ and $\epsilon_f+U_f\gg 0$ H_2 is simplified to

$$H_2=\frac{1}{2}\sum_k|V_k|^2\left[-\frac{1-f_k}{\epsilon_k-\epsilon_f}+\frac{f_k}{\epsilon_k-\epsilon_f-U_f}\right]$$
$$+\frac{1}{2L}\sum_{jkk'}V_kV_{k'}^{*}e^{i(k-k')\cdot r_j}\left[\frac{1}{\epsilon_k-\epsilon_f}-\frac{1}{\epsilon_k-\epsilon_f-U_f}\right]\boldsymbol{S}_j\cdot(c_k^{\dagger}\boldsymbol{\sigma}c_{k'})+\text{h.c.} \tag{A·5}$$

In the first term the conduction-electron number operator was replaced by the Fermi distribution function f_k. This term of the r.h.s. is just the second-order energy shift, which is always negative. The second term is the antiferromagnetic exchange coupling, which contains in general intersite terms; however the intersite contributions vanish when V_k is k-independent. Leaving the first term aside, we then obtain (1·2).

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