Paramagnons in heavy-electron systems

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(Received 30 October 1990; revised manuscript received 9 April 1991)

Paramagnons in heavy-electron systems are theoretically examined. First, local spin fluctuations are fully included in the best single-site approximation. A local Kondo temperature is uniquely defined to show a characteristic energy scale of local spin fluctuations. Secondly, paramagnons are included perturbatively. Such a theory is applied to analyze the specific-heat data of heavy-electron compounds such as UAl_2, UPt_3, and $CeSi_{1.85}$, where anomalous $T^3\ln T$ terms are observed at low temperatures $T<10$ K. It is argued that not only paramagnons but also local spin fluctuations are responsible for the low-temperature specific heat and that paramagnons are responsible for the anomalous $T^3\ln T$ terms.

I. INTRODUCTION

A certain class of lanthanide- and actinide-based compounds are called heavy-electron compounds, because their properties at low temperatures can be explained in terms of a Fermi liquid of extremely heavy quasiparticles.[1,2] Besides the large mass enhancement, they can also be characterized by the competition between the Kondo effect and the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction or by the competition between local and intersite spin fluctuations. Recent neutron-scattering experiments have clearly demonstrated the coexistence of both spin fluctuations.[3,4] A variety of low-temperature phases, such as normal Fermi liquids, superconducting states, and magnetic states, is easily understood if the competition is in a critical situation. When the RKKY exchange interaction is stronger than the Kondo effect, a compound should be paramagnetic, that is, a normal Fermi liquid or superconducting. Otherwise, it should be magnetic at low enough temperatures.

Because the number of f electrons per ion is very close to integer in any heavy-electron compound, they are also characterized by near localization of f electrons. It is reasonable that spin fluctuations are almost local as demonstrated by neutron scattering.[3,4] The large effective mass should be mainly due to local spin fluctuations, because their amplitude is large in the whole Brillouin zone, while the amplitude of intersite spin fluctuations is large only in a small part of the Brillouin zone. Therefore, it is expected that the single-site Kondo effect is a good starting point to include local spin fluctuations in certain heavy-electron compounds.[5] Such compounds are generally called Kondo lattices. Various treatments have already been proposed such as various extensions of results of the single-site Kondo effect,[6-8] the Gutzwiller method,[9,10] and auxiliary-particle (or slave-boson) method.[11-13]

By taking into account near localization, our strategy is similar to previous theories based on a single-site picture.[6-8] First, a heavy-electron liquid is constructed in the best single-site approximation (SSA) of the periodic Anderson model. The best SSA turns out to be the same problem as solving the corresponding Anderson model in both the real- and auxiliary-particle methods. However, this auxiliary-particle theory is distinct from the previous auxiliary-particle theories,[11-13] because *auxiliary particles themselves are confined and localized* as discussed in Secs. II and V. Local spin fluctuations are fully included in the best SSA, and a local Kondo temperature T_K is uniquely defined to show an energy scale of local spin fluctuations or the bandwidth of heavy electrons. Second, exchange interactions are included perturbatively. If the exchange interactions are sufficiently small compared with T_K, the perturbative treatment should be valid. The essentially same formulation, or its simpler version, has already been applied to magnetoresistance[14] and metamagnetic transitions[15] of heavy-electron systems, and to anomalous normal-state properties[16] and superconducting properties[17] of high-temperature (high-T_c) CuO_2 superconductors. In this paper another application is made to paramagnons in heavy-electron systems.

In several heavy-electron compounds such as UAl_2,[18,19] $CeSi_{2-x}$,[20] and UPt_3,[21] their specific heat at low temperatures such as $T<10$ K can be fitted in the well-known form predicted by the paramagnon theory:[22,23]

$$C-\beta T^3=\gamma T-\delta T^3\ln\frac{T_{\rm SF}}{T}+\cdots , \tag{1.1}$$

where the term βT^3 assigned to the phonon contribution should be subtracted from the observed specific heat C. Experimental γ, δ, and $T_{\rm SF}$ are listed in Table I. An energy scale $T_{\rm SF}$ is called the spin-fluctuation temperature of paramagnons. Because it is difficult to avoid small errors in subtracting the phonon contribution in Eq. (1.1), there must exist a small ambiguity in numbers of $T_{\rm SF}$ listed in Table I.

It is certain that a part of the specific heat below $T_{\rm SF}$, not only the anomalous logarithmic term, but also the large specific-heat coefficient γ, should be due to paramagnons, as argued by many groups.[1,2,18-21,24] However, there are no microscopic arguments on the competition between paramagnons and local spin fluctuations.

TABLE I. Observed γ, δ, and T_{SF}, of UAl_2, $CeSi_{1.85}$, and UPt_3.

	γ (expt.) [mJ/(mol K^2)]	δ (expt.) [mJ/(mol K^4)]	T_{SF} (expt.) (K)
UAl_2 (Ref. 19)	150	1.6	14
$CeSi_{1.85}$ (Ref. 20)	240	0.7	15
UPt_3 (Ref. 21)	420	1.4	15

In typical Kondo lattices such as CeB_6, $CeCu_6$, $CeSi_2Cu_2$, and so on, the electrical resistivity shows the well-known logarithmic increase in decreasing temperatures above local Kondo temperatures. However, no logarithmic increase has been observed in UAl_2, $CeSi_{1.85}$, and UPt_3, which are tentatively called spin fluctuators in this paper. Then it may be argued that Kondo lattices and spin fluctuators are qualitatively different in the nature of their electron correlation, as suggested by the logarithmic term of the resistivity. However, it may also be argued that they are qualitatively the same and that the difference is only quantitative. For example, it can be argued that T_K is lower than T_{SF} in Kondo lattices, while T_{SF} is lower than T_K in spin fluctuators. In any event, f electrons are almost localized in both classes of heavy-electron compounds, and f electrons are a little more itinerant in spin fluctuators than in Kondo lattices. To make a definite conclusion on this problem, both local spin fluctuations and paramagnons should be examined in a unified theoretical framework.

The purpose of this paper is to examine the specific heat of heavy-electron systems by including explicitly both local spin fluctuations and paramagnons. The plan of this paper is as follows: A new formulation in treating near-localized magnetism is presented in Sec. II. The theory is applied to paramagnons in heavy-electron systems in Sec. III. The observed specific heat of heavy-electron compounds is analyzed in Sec. IV. The difference between the other auxiliary-particle theories and the present theory is discussed in Sec. V. The paper is summarized in Sec. VI.

II. FORMULATION

A. Single-site approximation

Because heavy-electron systems have already been investigated in auxiliary-particle models,[11–13] we will also take an auxiliary-particle model to see the relation with other theories. Because auxiliary particles are just auxiliary, various auxiliary-particle models are possible. If the mapping between a real- and auxiliary-particle models is rigorously treated, however, they give the same results. Here we follow Barnes,[25] but we take a model with a slight modification to treat the mapping rigorously. The periodic Anderson model with a single f band is mapped to

$$\mathcal{H}=\sum_{n,ij,\sigma}(-\sigma\mu_B H\delta_{ij}+t_{n,ij})c^\dagger_{ni\sigma}c_{nj\sigma}+\sum_{i\sigma}(\varepsilon_f-\sigma\mu_B H)a^\dagger_{i\sigma}a_{i\sigma}+\sum_i \mu e^\dagger_i e_i$$
$$+\sum_i(2\varepsilon_f-\mu+U)d^\dagger_i d_i+\sum_{n,ij,\sigma}V_{ni,j}(c^\dagger_{ni\sigma}f_{j\sigma}+f^\dagger_{j\sigma}c_{ni\sigma})-\sum_i\lambda Q_i+\tfrac{1}{2}U_\infty\sum_i(Q_i-1)^2\ , \tag{2.1}$$

with

$$f^\dagger_{i\sigma}=e_i a^\dagger_{i\sigma}+\sigma a_{i-\sigma}d^\dagger_i \tag{2.2}$$

and

$$Q_i=a^\dagger_{i\uparrow}a_{i\uparrow}+a^\dagger_{i\downarrow}a_{i\downarrow}+e^\dagger_i e_i+d^\dagger_i d_i\ , \tag{2.3}$$

where $a^\dagger_{i\sigma}$, $e^\dagger_i$, and $d^\dagger_i$ are creation operators of auxiliary particles, with site i and spin σ; $c^\dagger_{ni\sigma}$ a creation operator of a conduction electron with band n, site i, and spin σ; ε_f the depth of f levels; $\mu_B H$ infinitesimally small Zeeman energy; U the on-site repulsion; and μ the chemical potential of electrons. Two or more than two conduction bands are assumed to make the system metallic without fail.

In this paper auxiliary particles are called a particles e particles and d particles. Sites occupied by f electrons are mapped to sites occupied by a particles, empty f sites to sites occupied by e particles, and doubly occupied f sites to sites occupied by d particles. Two types of statistics are possible in (2.1). In one method a particles are fermions, while e and d particles are bosons. In the other method, a particles are bosons, while e and d particles are fermions. The former method is used in this paper. Because f electrons themselves are mapped to fermionic pair excitations created by $f^\dagger_{i\sigma}$, they are called fermionic excitons or simply f electrons.

It is obvious that there exists a local argued symmetry

$$[\mathcal{H},Q_i]=0\ , \tag{2.4}$$

for any site i. Therefore, different subspaces $\{Q_i\}$ are disjoint to each other, unless the local gauge symmetry is broken. The mapping is rigorous only if the Hilbert space is restricted to

$$\{Q_i=1 \text{ for any sites}\}\ , \tag{2.5}$$

in (2.1). Therefore, the local gauge symmetry should never be broken. If the restriction (2.5) is rigorously taken into account, *any auxiliary particles are confined in the sense that no single-particle excitations of auxiliary particles are possible.* In order to argue their single-particle

excitations, the Hilbert space should be extended to

$$\{Q_i \neq 1 \quad \text{for some sites}\} \ . \tag{2.6}$$

Then the chemical potential λ of auxiliary particles can be introduced in (2.1) to satisfy

$$\sum_i \langle Q_i \rangle = N \ , \tag{2.7}$$

with $\langle Q_i \rangle$ the thermal average of Q_i and N the number of lattice sites. However, the Hamiltonian should be defined properly in the extended space (2.6) in order to exclude unphysical states and fluctuations. The last term with $U_\infty / U \to +\infty$ has been introduced in Eq. (2.1) to exclude unphysical states and fluctuations. Therefore, for example, either $\langle a_{i\sigma}^\dagger a_{j\sigma} \rangle$ with $i \neq j$, $\langle e_i^\dagger e_j \rangle$ with $i \neq j$, or $\langle d_i^\dagger d_j \rangle$ with $i \neq j$ can never be finite because of the local gauge symmetry (2.4). It means that *auxiliary particles themselves are localized in the sense that single-particle Green functions of auxiliary particles are site diagonal.*

Bare single-particle Green functions of auxiliary particles for $V_{ni,j}=0$ and $U_\infty = 0$ are given by

$$A_\sigma^{(0)}(i\varepsilon) = \frac{1}{i\varepsilon + \lambda - \varepsilon_f + \sigma\mu_B H} \ , \tag{2.8}$$

for a particles,

$$E^{(0)}(i\omega) = \frac{1}{i\omega + \lambda - \mu} \ , \tag{2.9}$$

for e particles, and

$$D^{(0)}(i\omega) = \frac{1}{i\omega + \lambda - 2\varepsilon_f + \mu - U} \ , \tag{2.10}$$

for d particles, respectively. Because they are localized, any single-particle Green functions of auxiliary particles are independent of sites or momenta.

Itinerant excitations are pair excitations such as fermionic excitons:

$$G_{ff\sigma}(i\varepsilon, \mathbf{k}) = \sum_j \int_0^{1/T} d\tau \exp[i\varepsilon\tau - i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)] G_{ij,\sigma}(\tau) \ , \tag{2.11}$$

with

$$G_{ij,\sigma}(\tau) = -\langle T_\tau f_{i\sigma}(\tau) f_{j\sigma}^\dagger \rangle \ . \tag{2.12}$$

Once the irreducible functions $K_\sigma(i\varepsilon, \mathbf{k})$ have been obtained, Green functions of fermionic excitons or f electrons are given by

$$G_{ff\sigma}(i\varepsilon, \mathbf{k}) = \left[K_\sigma^{-1}(i\varepsilon, \mathbf{k}) - \sum_n V_n^2(\mathbf{k}) C_{n\sigma}(i\varepsilon, \mathbf{k}) \right]^{-1} \ , \tag{2.13}$$

with

$$V_n(\mathbf{k}) = \frac{1}{N} \sum_{ij} V_{ni,j} \exp[i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)] \tag{2.14}$$

and

$$C_{n\sigma}(i\varepsilon, \mathbf{k}) = \frac{1}{i\varepsilon + \mu - \varepsilon_{n\sigma}(\mathbf{k})} \ , \tag{2.15}$$

with

$$\varepsilon_{n\sigma}(\mathbf{k}) = \frac{1}{N} \sum_{ij} t_{n,ij} \exp[i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)] - \sigma\mu_B H \ . \tag{2.16}$$

Other Green functions are given by

$$\begin{aligned} G_{fn\sigma}(i\varepsilon, \mathbf{k}) &= G_{nf\sigma}(i\varepsilon, \mathbf{k}) \\ &= C_{n\sigma}(i\varepsilon, \mathbf{k}) V_n(\mathbf{k}) G_{ff\sigma}(i\varepsilon, \mathbf{k}) \end{aligned} \tag{2.17}$$

and

$$\begin{aligned} G_{nm\sigma}(i\varepsilon, \mathbf{k}) &= \delta_{nm} C_{n\sigma}(i\varepsilon, \mathbf{k}) \\ &\quad + C_{n\sigma}(i\varepsilon, \mathbf{k}) V_n(\mathbf{k}) G_{ff\sigma}(i\varepsilon, \mathbf{k}) \\ &\quad \times V_m(\mathbf{k}) C_{m\sigma}(i\varepsilon, \mathbf{k}) \ , \end{aligned} \tag{2.18}$$

Let us examine $K_\sigma(i\varepsilon, \mathbf{k})$ in the perturbative treatment of $V_{ni,j}$ and U_∞. *All the skeleton diagrams are included, but the summation is restricted to the single-site diagrams in the SSA.* In any skeleton single-site diagram, lines of auxiliary particles have the same site index in a diagram. Therefore, $K_\sigma(i\varepsilon, \mathbf{k})$ is independent of $\mathbf{k}$ as $K_\sigma(i\varepsilon, \mathbf{k}) = K_\sigma(i\varepsilon)$ in the SSA. By following the usual diagrammatic method, every internal line is replaced by its renormalized line.

To sum up all the diagrams of $K_\sigma(i\varepsilon)$ in the SSA is the same problem as solving a certain single-site Anderson model:

$$\begin{aligned} \mathcal{H} &= \sum_{ij,\sigma} (-\sigma\mu_B H \delta_{ij} + \hat{t}_{ij,\sigma}) \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \\ &\quad + \sum_\sigma (\varepsilon_f - \sigma\mu_B H) \hat{a}_\sigma^\dagger \hat{a}_\sigma + \mu \hat{e}^\dagger \hat{e} + (2\varepsilon_f - \mu + U) \hat{d}^\dagger \hat{d} \\ &\quad + \sum_{i\sigma} \hat{V}_{i\sigma} (\hat{c}_{i\sigma}^\dagger \hat{f}_\sigma + \hat{f}_\sigma^\dagger \hat{c}_{i\sigma}) - \lambda \hat{Q} + \tfrac{1}{2} U_\infty (\hat{Q} - 1)^2 \ , \end{aligned} \tag{2.19}$$

with

$$\hat{f}_\sigma^\dagger = \hat{e} \hat{a}_\sigma^\dagger + \sigma \hat{a}_{-\sigma} \hat{d}^\dagger \tag{2.20}$$

and

$$\hat{Q} = \hat{a}_\uparrow^\dagger \hat{a}_\uparrow + \hat{a}_\downarrow^\dagger a_\downarrow + \hat{e}^\dagger \hat{e} + \hat{d}^\dagger \hat{d} \ , \tag{2.21}$$

where $\hat{c}_{i\sigma}^\dagger$, $\hat{a}_\sigma^\dagger$, $\hat{e}^\dagger$, and $\hat{d}^\dagger$ are creation operators of conduction electrons, with site i and spin σ, and auxiliary particles, respectively. The parameters μ, λ, ε_f, U, H, and U_∞ in Eq. (2.19) are the same as in the periodic model (2.1). The statistics of auxiliary particles is also the same between (2.1) and (2.19). Then we can write down each diagram of the irreducible function $\hat{K}_\sigma(i\varepsilon)$ of localized fermionic excitons or f electrons defined by

$$\hat{G}_\sigma(i\varepsilon) = -\int_0^{1/T} d\tau e^{i\varepsilon\tau} \langle T_\tau \hat{f}_\sigma(\tau) \hat{f}_\sigma^\dagger \rangle \ . \tag{2.22}$$

Once all the diagrams of $\hat{K}_\sigma(i\varepsilon)$ have been summed up, $\hat{G}_\sigma(i\varepsilon)$ is obtained as

$$\hat{G}_\sigma(i\varepsilon) = \left[\hat{K}_\sigma^{-1}(i\varepsilon) - \frac{1}{N} \sum_{\mathbf{k}} \frac{\hat{V}_\sigma^2(\mathbf{k})}{i\varepsilon + \mu - \hat{\varepsilon}_{c\sigma}(\mathbf{k})} \right]^{-1} \ , \tag{2.23}$$

with

$$\hat{\varepsilon}_{c\sigma}(\mathbf{k})=-\frac{1}{N}\sum_{ij}\hat{t}_{ij,\sigma}\exp[i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)]-\sigma\mu_B H \tag{2.24}$$

and

$$\hat{V}_\sigma(\mathbf{k})=\sum_i \hat{V}_{i\sigma}\exp[i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_0)]\ , \tag{2.25}$$

with $\mathbf{R}_0$ the impurity site.

Bare Green functions of auxiliary particles are the same between the two models. Therefore, it is easy to see that $K_\sigma(i\varepsilon)=\hat{K}_\sigma(i\varepsilon)$ if each line of renormalized conduction electrons in the impurity model is the same as a line of renormalized conduction electrons in the periodic model. The self-consistent condition of the SSA is

$$\frac{\hat{L}_\sigma(i\varepsilon)}{1-K_\sigma(i\varepsilon)\hat{L}_\sigma(i\varepsilon)}=R_\sigma(i\varepsilon)\ , \tag{2.26}$$

with

$$\hat{L}_\sigma(i\varepsilon)=\frac{1}{N}\sum_{\mathbf{k}}\frac{\hat{V}^2_\sigma(\mathbf{k})}{i\varepsilon+\mu-\hat{\varepsilon}_{c\sigma}(\mathbf{k})}\ , \tag{2.27}$$

in the impurity model, and

$$R_\sigma(i\varepsilon)=\frac{1}{N}\sum_{\mathbf{k}}\sum_{nm}V_n(\mathbf{k})G_{nm}(i\varepsilon,\mathbf{k})V_m(\mathbf{k})\ , \tag{2.28}$$

in the periodic model. Equation (2.26) shows what Anderson model should be solved self-consistently in the SSA. Therefore, not only $K_\sigma(i\varepsilon)=\hat{K}_\sigma(i\varepsilon)$ should be solved, but also the hybridization matrix defined by

$$\begin{aligned}\hat{\Delta}_\sigma(\varepsilon)&\equiv\pi\frac{1}{N}\sum_{\mathbf{k}}\delta(\varepsilon+\mu-\hat{\varepsilon}_{c\sigma}(\mathbf{k}))\hat{V}^2_\sigma(\mathbf{k})\\&=-\mathrm{Im}\left[\frac{R_\sigma(\varepsilon+i0)}{1+K_\sigma(\varepsilon+i0)R_\sigma(\varepsilon+i0)}\right]\\&=\mathrm{Im}\left[\left[\frac{1}{N}\sum_{\mathbf{k}}G_{ff\sigma}(\varepsilon+i0,\mathbf{k})\right]^{-1}-K^{-1}_\sigma(\varepsilon+i0)\right]\end{aligned} \tag{2.29}$$

should be determined self-consistently in the Anderson model (2.19). It is easy to see that the results do not depend on statistics of auxiliary particles.

Equation (2.26) or (2.29) is also equivalent with

$$\hat{G}_\sigma(i\varepsilon)=\frac{1}{N}\sum_{\mathbf{k}}G_{ff\sigma}(i\varepsilon,\mathbf{k})\ . \tag{2.30}$$

This is nothing but the SSA in the perturbative treatment in terms of U of real-particle models. Let us consider the self-energy $\Sigma_\sigma(i\varepsilon)$, which is related to $K_\sigma(i\varepsilon)$ as

$$\Sigma_\sigma(i\varepsilon)=-K^{-1}_\sigma(i\varepsilon)+i\varepsilon+\mu-\varepsilon_f+\sigma\mu_B H\ . \tag{2.31}$$

All the skeleton diagrams of $\Sigma_\sigma(i\varepsilon)$ are included in the SSA. In the SSA, however, the site indexes of the interaction lines U are restricted to the same site in a diagram. As a consequence, internal lines of electrons turn out to be site-diagonal lines. By following the usual diagrammatic method, each internal line is replaced by its renormalized line. Equation (2.30) requires that renormalized site-diagonal lines of the periodic Anderson model should be exactly the same as renormalized lines of the Anderson model. Therefore, to calculate $\Sigma_\sigma(i\varepsilon)$ in the SSA is the same problem as to calculate not only $\Sigma_\sigma(i\varepsilon)$, but also $\Delta_\sigma(i\varepsilon)$ self-consistently in the Anderson model. It is quite trivial that the self-consistent condition of the SSA does not depend on U_∞, because U_∞ appears only in the auxiliary-particle model. It is straightforward to see that even if any auxiliary-particle model is taken, the same self-consistent condition of the SSA as Eq. (2.30) is obtained.

Because the ground state of any impurity Anderson model is a normal Fermi liquid,[26–29] the ground state in the SSA is also a normal Fermi liquid. By using the results of the Anderson model,[28,29] $\Sigma_\sigma(i\varepsilon)$ can be expanded as

$$\begin{aligned}\Sigma_\sigma(i\varepsilon)=&\Sigma_0+(1-\phi_m)i\varepsilon+(1-\phi_s)\sigma\mu_B H\\&-(1-\phi_c)\Delta\varepsilon_f+\cdots\ ,\end{aligned} \tag{2.32}$$

with $\Delta\varepsilon_f$ infinitesimal variation of ε_f for $|i\varepsilon|\ll T_K$, and $|\mu_B H|\ll T_K$, where T_K is the local Kondo temperature which shows a characteristic energy scale of local spin fluctuations or the bandwidth of heavy electrons. According to Refs. 28 and 29,

$$T_K=\frac{\pi\hat{\Delta}_\sigma(0)}{4\phi_m}\ , \tag{2.33}$$

with $\phi_m\approx\frac{1}{2}\exp[U/\pi\hat{\Delta}_\sigma(0)]$ for the symmetric Anderson model with $U/\pi\hat{\Delta}_\sigma(0)\to+\infty$ and $n_f=1$, n_f being the number of f electrons per site. In an asymmetric Anderson model with $U/\pi\hat{\Delta}_\sigma(0)\to+\infty$ and $n_f<1$, $\phi_m\approx(\pi^2/8)/(1-n_f)$.[7] As long as $\phi_m\gg1$, a heavy-electron band is formed at the chemical potential.

Equation (2.30) shows that the density of states of f electrons in the SSA is the same as that of the impurity model. Therefore, it is obvious that the density of states of f electrons has three peaks in the SSA. One is a broadband around ε_f below the chemical potential, and another is a broadband around ε_f+U above the chemical potential. The other is the heavy-electron band at the chemical potential.

It is also straightforward to apply the best SSA to the Hubbard model, the real-particle Hubbard model, or any auxiliary-particle Hubbard model.[30,31] To calculate $\Sigma_\sigma(i\varepsilon)$ of the Hubbard model in the best SSA is the same problem as to calculate not only $\Sigma_\sigma(i\varepsilon)$, but also $\hat{\Delta}_\sigma(i\varepsilon)$ self-consistently in the Anderson model. The self-consistent condition of the SSA is that, in the expression of the real-particle model, renormalized site-diagonal lines of the Hubbard model should be exactly the same as renormalized lines of the Anderson model. Therefore, the existence of conduction electrons is not necessarily relevant for the formation of heavy electrons.

By following Luttinger,[32] it can be proved that the Fermi-liquid relations should be satisfied within the SSA. The specific-heat coefficient is given by

$$\gamma_{\mathrm{loc}}=\frac{1}{3}\pi^2k_B^2\frac{1}{N}\sum_{\mathbf{k}\sigma}\left[-\frac{1}{\pi}\right]\mathrm{Im}\left[\phi_m G_{ff\sigma}(+i0,\mathbf{k})+\sum_n G_{nn\sigma}(+i0,\mathbf{k})\right]\ , \tag{2.34}$$

with k_B the Boltzmann constant. The Fermi-surface sum rule at $T=0$ K is given by

$$n_\sigma=\frac{1}{N}\sum_{\mathbf{k}}\left[-\frac{1}{\pi}\right]\mathrm{Im}\left[\ln[-1/G_{ff\sigma}(+i0,\mathbf{k})]+\sum_n \ln[-1/C_{n\sigma}(+i0,\mathbf{k})]\right], \tag{2.35}$$

the spin susceptibility at $T=0$ K by

$$\chi_s^{(0)}(i\omega=0,|\mathbf{q}|\to 0)=\frac{\partial(n_\uparrow-n_\downarrow)}{\partial(\mu_B H)}=\frac{1}{N}\sum_{\mathbf{k}\sigma}\left[-\frac{1}{\pi}\right]\mathrm{Im}\left[\phi_s G_{ff\sigma}(+i0,\mathbf{k})+\sum_n G_{nn\sigma}(+i0,\mathbf{k})\right], \tag{2.36}$$

and the charge susceptibility at $T=0$ K by

$$\chi_c^{(0)}(i\omega=0,\ |\mathbf{q}|\to 0)=\frac{\partial(n_\uparrow+n_\downarrow)}{\partial(\Delta\mu)}=\frac{1}{N}\sum_{\mathbf{k}\sigma}\left[-\frac{1}{\pi}\right]\mathrm{Im}\left[\phi_c G_{ff\sigma}(+i0,\mathbf{k})+\sum_n G_{nn\sigma}(+i0,\mathbf{k})\right]. \tag{2.37}$$

In the auxiliary-particle model, perturbations are not applied to f electrons, but to auxiliary particles. Therefore, vertex functions should be evaluated to argue low-energy phenomena in terms of f electrons. Vertex functions can be obtained by taking the derivative of the Green functions of f electrons:

$$\frac{\partial G_{ff\uparrow}(i\varepsilon,\mathbf{k})}{\partial(\mu_B H)}=-G_{ff\uparrow}^2(i\varepsilon,\mathbf{k})\frac{\partial K_\uparrow^{-1}(i\varepsilon)}{\partial(\mu_B H)}\ . \tag{2.38}$$

Therefore, vertex functions to exchange interactions are given by

$$\Gamma_s(i\varepsilon,i\omega=0)=\frac{\partial K_\uparrow^{-1}(i\varepsilon)}{\partial(\mu_B H)}=\phi_s\ , \tag{2.39}$$

in the limit of small transferred frequencies. By using the isotropic property in the absence of magnetic fields, $\Gamma_s=\phi_s$ can be used even for transverse processes. Similarly, vertex functions to charge-charge couplings are given by ϕ_c. However, ϕ_c is much smaller than ϕ_s, that is, $\phi_c \ll 1 \ll \phi_s$ in strong correlation regime. The Wilson ratio is almost as large as 2;[28,29]

$$W=\frac{\phi_s}{\phi_m}\approx 2\ , \tag{2.40}$$

as long as charge fluctuations are so suppressed such that $\phi_c \ll 1$.

As far as we are concerned with low-energy phenomena, Green functions of electrons can be approximately expressed as

$$G_{ff\sigma,\alpha}(i\varepsilon,\mathbf{k})=\frac{1}{Z_m(\mathbf{k})}\frac{1}{i\varepsilon-\varepsilon^*_{\alpha\sigma}(\mathbf{k})}\ , \tag{2.41}$$

$$G_{fn\sigma,\alpha}(i\varepsilon,\mathbf{k})=G_{nf\sigma,\alpha}(i\varepsilon,\mathbf{k})=Y_n(\mathbf{k})G_{ff\sigma,\alpha}(i\varepsilon,\mathbf{k})\ , \tag{2.42}$$

and

$$G_{nm\sigma,\alpha}(i\varepsilon,\mathbf{k})=Y_n(\mathbf{k})Y_m(\mathbf{k})G_{ff\sigma,\alpha}(i\varepsilon,\mathbf{k})\ , \tag{2.43}$$

with

$$Y_n(\mathbf{k})=V_n(\mathbf{k})C_{n\sigma}(+i0,\mathbf{k}) \tag{2.44}$$

and

$$Z_m(\mathbf{k})=\phi_m+\sum_n Y_n^2(\mathbf{k})\approx\phi_m\ . \tag{2.45}$$

Here $\varepsilon^*_{\alpha\sigma}(\mathbf{k})$ is the dispersion relation of heavy electrons defined by the real part of the αth pole of $G_{ff\sigma}(i\varepsilon,\mathbf{k})$:

$$\varepsilon^*_{\alpha\sigma}(\mathbf{k})=\mathrm{Re}(z_\alpha)\ , \tag{2.46}$$

where z_α is the pole defined by

$$1/G_{ff\sigma}(z_\alpha,\mathbf{k})=0\ . \tag{2.47}$$

Dynamical spin susceptibilities of f electrons are approximately obtained as

$$\chi_f^{(0)}(i\omega,\mathbf{q})=-\frac{1}{N}\sum_{\alpha\mathbf{k}\sigma}T\sum_{i\varepsilon}\phi_s^2 G_{ff\sigma,\alpha}(i\varepsilon+i\omega,\mathbf{k}+\tfrac{1}{2}\mathbf{q})G_{ff\sigma,\alpha}(i\varepsilon,\mathbf{k}-\tfrac{1}{2}\mathbf{q})=W^2\Pi(i\omega,\mathbf{q})\ , \tag{2.48}$$

with

$$\Pi(i\omega,\mathbf{q})=\frac{1}{N}\sum_{\alpha\mathbf{k}\sigma}\frac{f(\varepsilon^*_{\alpha\sigma}(\mathbf{k}-\mathbf{q}/2))-f(\varepsilon^*_{\alpha\sigma}(\mathbf{k}+\mathbf{q}/2))}{\varepsilon^*_{\alpha\sigma}(\mathbf{k}+\mathbf{q}/2)-\varepsilon^*_{\alpha\sigma}(\mathbf{k}-\mathbf{q}/2)-i\omega}\ , \tag{2.49}$$

the polarization function of heavy electrons with

$$f(\varepsilon)=\frac{1}{\exp(\varepsilon/T)+1}\ . \tag{2.50}$$

Interband contributions have been ignored in Eq. (2.48), because we are concerned with low-energy phenomena such as $|i\omega| \ll T_K$. The contribution by conduction elec-

trons is small enough to be ignored in strongly correlated systems. In the limit of $\omega=0$ and $|\mathbf{q}|\to 0$, the real part of Eq. (2.48) is about W times as large as the first term of Eq. (2.36), which is rigorous within the SSA. The present method will give the correct magnitude as far as we are concerned with the ω-linear imaginary part, because Shiba's argument[33] for the impurity Anderson model is also applied to the periodic model. Therefore,

$$\chi_f^{(0)}(\omega+i0,\mathbf{q})=W\,\mathrm{Re}[\Pi(\omega+i0,\mathbf{q})] +iW^2\mathrm{Im}[\Pi(\omega+i0,\mathbf{q})] \tag{2.51}$$

will be used as the susceptibility due to f electrons.

The specific-heat coefficient γ_{loc} given by Eq. (2.34) is simply expressed by

$$\gamma_{\mathrm{loc}}=\frac{2}{3}\pi^2 k_B^2\rho^*(0)\ , \tag{2.52}$$

with

$$\rho^*(\varepsilon)=\frac{1}{N}\sum_{\alpha\mathbf{k}}\delta(\varepsilon-\varepsilon^*_{\alpha\sigma}(\mathbf{k}))\ , \tag{2.53}$$

the density of states of heavy electrons. When we assume a single band of heavy electrons with the dispersion relation given by

$$\varepsilon^*_\sigma(\mathbf{k})=\frac{\hbar^2k^2}{2m^*}+\mathrm{const}\ , \tag{2.54}$$

the density of states at the chemical potential is given by

$$\rho^*(0)=\frac{3}{4}\frac{1}{k_BT_F^*}\ . \tag{2.55}$$

Therefore, the specific-heat coefficient due to local spin fluctuations is given by

$$\gamma_{\mathrm{loc}}=\frac{1}{2}\pi^2k_B\frac{1}{T_F^*}\ , \tag{2.56}$$

in this simple model. Because the specific-heat coefficient is given by

$$\hat{\gamma}=\frac{1}{6}\pi^2k_B\frac{1}{\hat{T}_K}\ , \tag{2.57}$$

in the Kondo effect with Kondo temperature $\hat{T}_K$ the local Kondo temperatures T_K is approximately given by

$$T_K=\tfrac{1}{3}T_F^*\ . \tag{2.58}$$

The susceptibility due to f electrons is expanded as

$$\chi_f^{(0)}(\omega+i0,\mathbf{q}) =2W\rho^*(0)\left\{1+r\left[-\frac{1}{3}\left[\frac{q}{2k_F}\right]^2-\left[\frac{\omega}{\hbar v_Fq}\right]^2\right] +i\pi W\frac{\omega}{\hbar v_Fq}+\cdots\right\}, \tag{2.59}$$

with

$$v_F=\frac{\hbar k_F}{m^*}\ , \tag{2.60}$$

the renormalized Fermi velocity. Because the Fermi-liquid relation [Eq. (2.36)] tells nothing about the expansion coefficients of the real part for finite ω and finite $\mathbf{q}$, a numerical factor r of the order of unity is assumed in Eq. (2.59). The imaginary part of Eq. (2.59) vanishes outside the regime of

$$\frac{\omega}{2\hbar k_Fv_F}<\frac{q}{2k_F}-\left[\frac{q}{2k_F}\right]^2\ . \tag{2.61}$$

B. c-f and RKKY exchange interactions

Local spin fluctuations are fully included in the best SSA. However, any intersite couplings between local spin fluctuations are ignored in the SSA. Therefore, the SSA is nothing but the random-phase approximation (RPA) in real space. Intersite couplings are examined in this subsection. The c-f exchange interaction can be derived by the virtual exchange process of a single e or d particle.[30,31] The matrix element is given by

$$-\sum_{nm}\sum_{ijj'}\sum_{\eta}\sum_{\substack{\alpha\beta\\ \gamma\delta}}(J_e^{(i;nj,mj')}+J_d^{(i;nj,mj')})(\tfrac{1}{2}\sigma_\eta^{\alpha\beta})(\tfrac{1}{2}\sigma_\eta^{\gamma\delta})\langle\langle a_{i\alpha}^\dagger a_{i\beta}c_{nj\gamma}^\dagger c_{mj'\delta}\rangle\rangle\ , \tag{2.62}$$

with

$$\sigma_x=\begin{bmatrix}0&1\\1&0\end{bmatrix},\quad \sigma_y=\begin{bmatrix}0&-i\\i&0\end{bmatrix}\quad\text{and}\quad \sigma_z=\begin{bmatrix}1&0\\0&-1\end{bmatrix},$$

$$J_e^{(i;nj,mj')}=-4V_{nj,i}V_{mj',i}E^{(0)}(\varepsilon_f-\lambda) \tag{2.63}$$

$$=-4V_{nj,i}V_{mj',i}\frac{1}{\mu-\varepsilon_f}\ , \tag{2.64}$$

and

$$J_d^{(i;nj,mj')}=-4V_{nj,i}V_{mj',i}D^{(0)}(\varepsilon_j-\lambda) =-4V_{nj,i}V_{mj',i}\frac{1}{U-\mu+\varepsilon_f}\ . \tag{2.65}$$

Operators in the double brackets, have been shown in Eq. (2.62) to show outgoing and incoming particles. Any charge-charge couplings have been ignored in Eq. (2.62). The c-f exchange interaction (2.62) due to virtual exchange of a confined and localized e or d particle is dis-

tinct from quasiparticle interactions due to virtual exchange of itinerant auxiliary particles, that is, effective hybridization fluctuations[11] or density fluctuations.[34]

The second-order perturbation of the c-f exchange interaction gives the RKKY exchange interaction between a particles:

$$J_{\mathrm{RKKY}}(i\omega,\mathbf{q})=J_{\mathrm{intra}}(i\omega,\mathbf{q})+J_{\mathrm{inter}}(i\omega,\mathbf{q})-J_0(i\omega)\ , \tag{2.66}$$

where

$$J_{\mathrm{intra}}(i\omega,\mathbf{q})=\frac{1}{4\phi_m^2}\frac{1}{N}\sum_{\alpha\mathbf{k}\sigma}M(\mathbf{k},\mathbf{q})\frac{f(\varepsilon^*_{\alpha\sigma}(\mathbf{k}-\mathbf{q}/2))-f(\varepsilon^*_{\alpha\sigma}(\mathbf{k}+\mathbf{q}/2))}{\varepsilon^*_{\alpha\sigma}(\mathbf{k}+\mathbf{q}/2)-\varepsilon^*_{\alpha\sigma}(\mathbf{k}-\mathbf{q}/2)-i\omega}\ , \tag{2.67}$$

with

$$M(\mathbf{k},\mathbf{q})=16\left[\frac{1}{\mu-\varepsilon_f}+\frac{1}{U-\mu+\varepsilon_f}\right]^2\sum_{nm}V_n^2(\mathbf{k}+\tfrac{1}{2}\mathbf{q})Y_n(\mathbf{k}+\tfrac{1}{2}\mathbf{q})V_m^2(\mathbf{k}-\tfrac{1}{2}\mathbf{q})Y_m(\mathbf{k}-\tfrac{1}{2}\mathbf{q})\ , \tag{2.68}$$

is the intraband contribution, while $J_{\mathrm{inter}}(i\omega,\mathbf{q})$ is the interband contribution. The on-site parts of the c-f exchange interaction have already been included in the SSA, because what realize heavy electrons are nothing but its on-site parts. Therefore,

$$J_0(i\omega)=\frac{1}{N}\sum_{\mathbf{q}}[J_{\mathrm{intra}}(i\omega,\mathbf{q})+J_{\mathrm{inter}}(i\omega,\mathbf{q})] \tag{2.69}$$

has been subtracted in Eq. (2.66) in order to exclude the on-site contribution, and

$$\sum_{\mathbf{q}}J_{\mathrm{RKKY}}(i\omega,\mathbf{q})=0\ . \tag{2.70}$$

If the nesting of the Fermi surface is significant, which gives a large peak of $J_{\mathrm{RKKY}}(0,\mathbf{q})$ at finite $\mathbf{q}$, $J_{\mathrm{RKKY}}(0,0)$ can be negative. However, it is obvious that

$$J_{\mathrm{RKKY}}(0,0)>0\ , \tag{2.71}$$

in two or three dimensions, if the dispersion relation Eq. (2.54) is assumed. Therefore, it is likely that the homogeneous part of the exchange interaction is positive in many compounds. Positive $J_{\mathrm{RKKY}}(0,0)$ can cause the paramagnon effect. It should be noted that

$$J_{\mathrm{intra}}\propto 1/\phi_m \quad\text{and}\quad J_{\mathrm{inter}}\propto(1/\phi_m)^0\ , \tag{2.72}$$

because excitations with large energies contribute to the interband term. If the interband contribution can be ignored, the RKKY exchange interaction is approximately proportional to local Kondo temperature. Therefore, one-parameter scaling[35,36] in the metamagnetic transition of $CeRu_2Si_2$ can be easily explained, if the RKKY exchange interaction comes mainly from intraband contributions.

By assuming the dispersion relation of heavy electrons given by Eq. (2.54), $J_{\mathrm{RKKY}}(\omega+i0,\mathbf{q})$ can also be expanded for small ω and $\mathbf{q}$ as

$$J_{\mathrm{RKKY}}(\omega+i0,\mathbf{q})=J_{\mathrm{RKKY}}(0,0)\left\{1-jr\left[\frac{1}{3}\left[\frac{q}{2k_F}\right]^2+\left[\frac{\omega}{\hbar v_F q}\right]^2\right]+i\pi jW\frac{\omega}{\hbar v_F q}+\cdots\right\}\ , \tag{2.73}$$

with j a numerical constant of the order of unity. Here the dependences of the interband term $J_{inter}(\omega+i0,\mathbf{q})$ on ω or $\mathbf{q}$ have been ignored.

III. SPECIFIC HEAT DUE TO PARAMAGNONS

By treating the RKKY exchange interaction in the conventional RPA in momentum space, the dynamical susceptibility can be calculated as

$$\chi_s(\omega+i0,\mathbf{q})=\frac{\chi_f^{(0)}(\omega+i0,\mathbf{q})}{1-\frac{1}{4}J_{\mathrm{RKKY}}(\omega+i0,\mathbf{q})\chi_f^{(0)}(\omega+i0,\mathbf{q})}\ . \tag{3.1}$$

Therefore, the stability condition of normal heavy electrons against magnetism is given by

$$\tfrac{1}{4}J_{\mathrm{RKKY}}(0,\mathbf{q})<T_K\ , \tag{3.2}$$

for any $\mathbf{q}$ by using Eqs. (2.55), (2.58), and (2.59). In the zeroth approximation $J_{\mathrm{RKKY}}(0,\mathbf{q})$ is roughly proportional to T_K, as can be seen from Eq. (2.72). Therefore, normal heavy electrons must be more stable than predicted by previous theories.[9,37] The stability of normal Kondo lattices depends on band structure or the nesting of the Fermi surface. The renormalization of heavy electrons in the SSA by intersite spin fluctuations is relatively small, as long as Eq. (3.2) is satisfied. Therefore, the RPA in momentum space is valid in the regime (3.2). The static homogeneous susceptibility can be expressed as

$$\chi_s(0,|\mathbf{q}|\to 0)=\frac{2W\rho^*(0)}{1-\alpha}\ , \tag{3.3}$$

with

$$\alpha=\tfrac{1}{2}J_{\mathrm{RKKY}}(0,0)W\rho^*(0)\ . \tag{3.4}$$

In the RPA, as in the original paramagnon theory,[24,25] the correction to the free energy by the RKKY exchange interaction is calculated as

$$\Delta\Omega(T)=\frac{3}{2}\int_{-\infty}^{+\infty}d\omega\coth\left[\frac{\omega}{2k_BT}\right]\frac{1}{2\pi N}\sum_{\mathbf{q}}\mathrm{Im}\left[\ln\left[1-\frac{1}{4}J_{\mathrm{RKKY}}(\omega+i0,\mathbf{q})\chi_f^{(0)}(\omega+i0,\mathbf{q})\right]\right] \tag{3.5a}$$

$$=\frac{3}{4\pi^3}\int_0^{\hbar v_F q_c}\coth\left[\frac{\omega}{2k_BT}\right]\int_{\omega/\hbar v_F}^{q_c}dq\,q^2\tan^{-1}\left[\frac{(\pi/2)(W/r)(\omega/\hbar v_F q)}{A+\frac{1}{3}(q/2k_F)^2+(\omega/\hbar v_F q)^2}\right], \tag{3.5b}$$

with

$$A=\frac{1-\alpha}{\alpha(1+j)r}\ . \tag{3.6}$$

The inverse of A can be regarded as an enhancement factor. The factor $\frac{3}{2}$ in Eq. (3.5) comes from the contributions of the longitudinal spin fluctuations as well as the transverse spin fluctuations. It can be easily seen from the susceptibility (3.3) that when the system is very close to ferromagnetic instability, the factor A is much smaller than unity.

Because of Eq. (2.70), the real part of $J_{\mathrm{RKKY}}(\omega+i0,\mathbf{q})$ can never be positive in the whole region of the Brillouin zone. The integration over $\mathbf{q}$ in Eq. (3.5a) can only have significant contributions in the region where $\mathrm{Re}[J_{\mathrm{RKKY}}(\omega+i0,\mathbf{q})]$ is positive and spin fluctuations are well developed. Therefore, the cutoff of the momentum integration is naturally introduced in Eq. (3.5a). The feature is in clear contrast with the cutoff $q_c\approx 2k_F$ in the original paramagnon theory.[22,23] Because expansion forms are used, however, a phenomenological cutoff q_c is introduced in Eq. (3.5b). In Eq. (3.5b) the integration over $\mathbf{q}$ should be restricted, at least to the region where $\mathrm{Re}[J_{\mathrm{RKKY}}(\omega+i0,\mathbf{q})]$ is positive. For example,

$$y_c\equiv\frac{q_c}{2k_F}\approx 0.5\ , \tag{3.7}$$

if it is assumed that there exists a single Fermi surface and that $\mathrm{Re}[J_{\mathrm{RKKY}}(\omega+i0,\mathbf{q})]$ is positive in about a half of the Brillouin zone around $\mathbf{q}=\mathbf{0}$. Because it depends on band structure, the cutoff q_c or y_c is left as a parameter to be determined experimentally in the present paper.

The upper limit of the ω integration and the lower limit of the q integration in Eq. (3.5b) come from the restriction that the imaginary parts of Eqs. (2.59) and (2.73) are nonzero in the region of Eq. (2.61). Because the main contribution of Eq. (3.5) comes from the region

$$\frac{\omega}{\hbar k_F v_F}\ll 1\ , \tag{3.8}$$

Eq. (3.8) is assumed to set the lower limit of the q integration.

The specific heat due to paramagnons is given by

$$\frac{\Delta C}{T}=-\frac{\partial^2\Delta\Omega(T)}{\partial T^2}$$

$$=\frac{3}{4\pi^3}k_B^2\int_0^{\hbar v_F q_c}d\omega\,G\left[\frac{\omega}{2k_BT}\right]\int_{\omega/\hbar v_F}^{q_c}dq\,q^2\tan^{-1}\left[\frac{(\pi/2)(W/r)(\omega/\hbar v_F q)}{A+\frac{1}{3}(q/2k_F)^2+(\omega/\hbar v_F q)^2}\right], \tag{3.9}$$

with

$$G(x)=2x\frac{d}{dx}g(x)+x^2\frac{d^2}{dx^2}g(x)\ , \tag{3.10}$$

with

$$g(x)=\frac{1}{\exp(x)-1}\ . \tag{3.11}$$

By making use of relations

$$\int_0^{+\infty}dx\,xG(x)=\frac{\pi^2}{3} \tag{3.12}$$

and

$$\int_0^{+\infty}dx\,x^3G(x)=\frac{4\pi^4}{5}\ , \tag{3.13}$$

the asymptotic form of Eq. (3.9) at low temperatures can be calculated as

$$\frac{\Delta C}{T}=\gamma_p-\delta T^2\ln\frac{T_{\mathrm{SF}}}{T}+\cdots\ , \tag{3.14}$$

with

$$\gamma_p=\frac{9}{4}\frac{W}{r}\frac{\pi^2k_B}{T_F^*}\ln\left[1+\frac{y_c^2}{3A}\right], \tag{3.15}$$

the linear specific-heat coefficient,

$$T_{\mathrm{SF}}=\theta A^{3/2}T_F^*\ , \tag{3.16}$$

with θ a constant of the order of unity, which depends on y_c and A, and

$$\delta=\frac{3\pi^6}{160}\left[\left[\frac{W}{r}\right]^3+\frac{W}{r}\frac{12A}{\pi^2}\right]\frac{k_B}{T_p^3}\ , \tag{3.17}$$

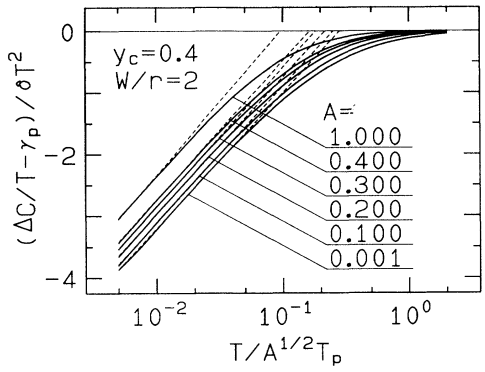

FIG. 1. $(\Delta C-\gamma_p)/\delta T^2$ as a function of $\ln(T/A^{1/2}T_p)$ for $y_c=0.4$ and various A. Dotted lines express the asymptotic expressions.

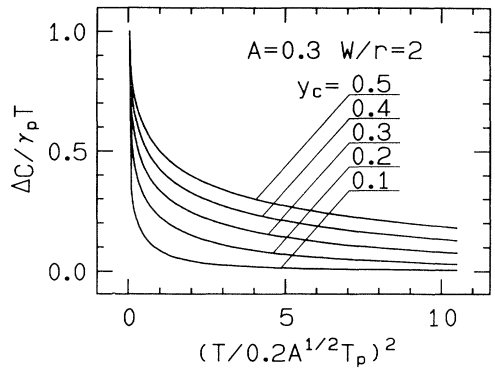

FIG. 3. $\Delta C/\gamma_p$ as a function of $(T/0.2A^{1/2}T_p)^2$ for $A=0.3$ and various y_c. The spin-fluctuation temperature of paramagnons is approximately given by $T_{\rm SF}\approx 0.2A^{1/2}T_p$.

with

$$T_p = AT_F^* \ . \tag{3.18}$$

The mass enhancement due to paramagnons is large for

$$\frac{y_c^2}{3A} \gg 1 \ , \tag{3.19}$$

that is, when the enhancement factor $1/A$ is large and paramagnons are widely extended in the Brillouin zone. The second term proportion to $(W/r)(A/T_p^3)$ in Eq. (3.17) is new. However, it can be ignored, unless the factor A is as large as unity.

At elevated temperatures the contribution of paramagnons can be numerically calculated. Figure 1 shows

$$\left[\frac{\Delta C}{T}-\gamma_p\right]\frac{1}{\delta T^2} \ , \tag{3.20}$$

as a function of

$$\ln(T/A^{1/2}T_p) \ , \tag{3.21}$$

for $y_c=0.4$, $W/r=2$, and various A, while Fig. 2 shows

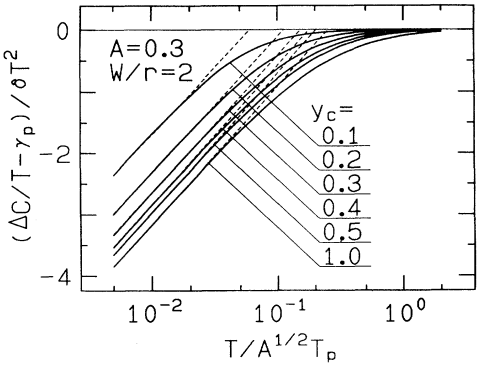

FIG. 2. $(\Delta C-\gamma_p)/\delta T^2$ as a function of $\ln(T/A^{1/2}T_p)$ for $A=0.3$ and various y_c.

the same quantity for $A=0.3$, $W/r=2$, and various y_c. It can be seen from these figures that the dependences of θ on A and y_c are small for

$$A \lesssim 0.4 \quad \text{and} \quad y_c \gtrsim 0.3 \ . \tag{3.22}$$

Therefore, we obtain

$$\theta \approx 0.2 \quad \text{and} \quad T_{\rm SF}\approx 0.2A^{1/2}T_p \ , \tag{3.23}$$

in the region of Eq. (3.22).

The asymptotic form (3.14) can only be used at low temperatures. The constant θ depends on parameters such as A, y_c, and W/r. However, once $T_{\rm SF}$ is given, the asymptotic expression (3.14) can be approximately used at temperatures such as

$$T < 0.5T_{\rm SF} \tag{3.24}$$

and precisely used at

$$T < 0.3T_{\rm SF} \ , \tag{3.25}$$

in any cases. This feature is consistent with numerical results by a phenomenological theory of paramagnons.[38] Figure 3 shows $\Delta C/\gamma_p T$ as a function of

$$(T/0.2A^{1/2}T_p)^2 \ . \tag{3.26}$$

It can be seen that the specific heat due to paramagnons becomes small above the spin fluctuation temperature $T_{\rm SF}$ for $A=0.3$ and $y_c<0.5$. On the other hand, their contribution is still large above $T_{\rm SF}$ for very small A and large y_c.

IV. APPLICATION TO HEAVY-ELECTRON COMPOUNDS

By taking the numbers of T_F and T_p in units of Kelvin, various numbers can be calculated as

$$\gamma_{\rm loc}=4.10\times 10^4\frac{1}{T_F^*}\ \text{mJ/(mol K}^2) \ , \tag{4.1}$$

$$\gamma_p = 6.15\times10^4 \frac{y_c^2}{T_p}\frac{W}{r}\ \mathrm{MJ/(mol\,K^2)}$$
$$= 1.23\times10^5 \frac{y_c^2}{T_p}\ \mathrm{mJ/(mol\,K^2)}\ , \tag{4.2}$$

and

$$\delta = 1.50\times10^5 \frac{1}{T_p^3}\left[\frac{W}{r}\right]^3\ \mathrm{mJ/(mol\,K^4)}$$
$$= 1.20\times10^6 \frac{1}{T_p^3}\ \mathrm{mJ/(mol\,K^4)}\ , \tag{4.3}$$

where

$$\frac{W}{r}=2,\quad \left[\frac{r}{W}\right]^2 A \ll 1\ ,\ \text{and}\ \frac{y_c^2}{3A}\ll 1 \tag{4.4}$$

are assumed.

What should be first in analyzing the experimental data is to divide the observed γ listed in Table I into γ_{loc} and γ_p. We will do it crudely. For example, Fig. 4 shows the experimental C/T as a function of T^2 of UPt_3.[21] As discussed below, impurities suppress the logarithmic term. Therefore, the phonon part $\Delta C_{\mathrm{ph}}/T=\beta T^2$ with

$$\beta = 0.8\ \mathrm{mJ/(mol\,K^4)} \tag{4.5}$$

is assumed from alloyed compounds $UPt_{3-x}Pd_x$.[39] By taking into account that $\Delta C/T$ due to paramagnons at T_{SF} is about a half of $\Delta C/T$ at $T=0$ K, as shown in Fig. 3, we can draw a dashed line in Fig. 4, which is assumed to be the sum of γ_{loc} and $\Delta C_{\mathrm{ph}}/T=\beta T^2$. Then we obtain

$$\gamma_{\mathrm{loc}} \approx 150\ \mathrm{mJ/(mol\,K^2)} \tag{4.6}$$

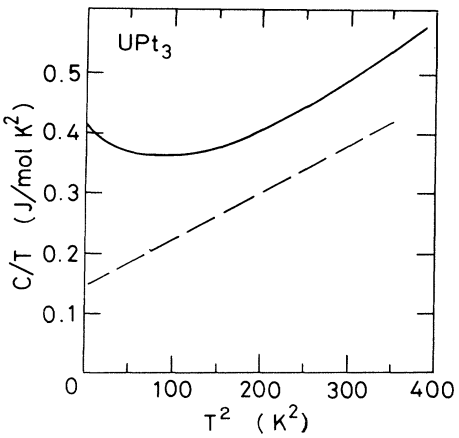

FIG. 4. Specific heat C/T of UPt_3 as a function of T^2. The solid line is an experimental result of Ref. 21, and the dashed line is assumed to be due to local spin fluctuations and phonons, $\gamma_{\mathrm{loc}}+\beta T^2$, where $\beta=0.79$ mJ/(mol K^4) is taken from alloyed samples $UPt_{3-x}Pd_x$ of Ref. 39. Then the linear specific-heat coefficient γ is divided into γ_{loc} due to local spin fluctuations and γ_p due to paramagnons.

and

$$\gamma_p \approx 270\ \mathrm{mJ/(mol\,K^2)}\ , \tag{4.7}$$

ignoring the contributions of antiferromagnetic fluctuations, which are observed by neutron scattering.[3,4] Equation (4.6) gives

$$T_F^* \approx 270\ \mathrm{K}\ \text{or}\ T_K \approx 90\ \mathrm{K}\ , \tag{4.8}$$

and Eq. (4.7) gives

$$\frac{T_p}{y_c^2} \approx 460\ \mathrm{K}\ . \tag{4.9}$$

On the other hand, the experimental δ about 1.4 mJ/(mol K^4) gives

$$T_p \approx 95\ \mathrm{K}\ . \tag{4.10}$$

From Eqs. (3.18) and (4.8)–(4.10), the parameters in the paramagnon theory are calculated as

$$A \approx 0.35\ \text{and}\ y_c \approx 0.46\ . \tag{4.11}$$

From the values of A and T_p, the spin fluctuation temperature is calculated from Eq. (3.23) as

$$T_{\mathrm{SF}} \approx 15\ \mathrm{K}\ , \tag{4.12}$$

by assuming $\theta=0.2$. This number is listed in Table II, and it should be compared with the experimental number of $T_{\mathrm{SF}}\approx 15$ K listed in Table I. The same analysis can be made for UAl_2 of Ref. 19 and $CeSi_{1.85}$ of Ref. 20. Figure 5 shows the experimental C/T as a function of T^2 of UAl_2.[19] The estimated numbers are also shown in Table II.

Many features should be included to make analyses of the specific heat in detail such as band-structure effects, the specific heat due to antiferromagnetic spin fluctuations, the term of the specific heat proportional to T^3 due to local spin fluctuations, and so on. However, the analyses give an agreement between the experimental T_{SF} and theoretical T_{SF}, in particular, for $CeSi_{1.85}$ and UPt_3. The experimental values of y_c are not inconsistent with a rough value given by Eq. (3.7). Therefore, it is likely that paramagnons are responsible for the observed $T^3\ln T$ term of $CeSi_{1.85}$ and UPt_3, and that they are at least responsible for a part of the upturn of the specific heat at low temperatures of UAl_2.

The energy scales are different between local spin fluctuations and paramagnons as

$$T_{\mathrm{SF}} \ll T_F^*\ . \tag{4.13}$$

This implies that typical Fermi-liquid behaviors can only be expected below $T_{\mathrm{SF}}\approx 10$ K and that spin fluctuations of paramagnons should behave like localized moments above T_{SF}, for example, in the nuclear magnetic relaxation rate. The situation seems to be similar to antiferromagnetic fluctuations in the high-T_c CuO_2 superconductors, where typical Fermi-liquid behaviors can only be expected below a characteristic temperature $T_a\approx 100$ K of antiferromagnetic fluctuations.[16]

In actual spin fluctuators, the logarithmic $T^3\ln T$ term

TABLE II. Estimated parameters according to the present theory. The theoretical T_{SF} in this table should be compared to the experimental T_{SF} in Table I.

	γ_{loc} [mJ/(mol K^2)]	γ_p [mJ/(mol K^2)]	T_F^* (K)	T_p (K)	A	y_c	T_{SF} (K)	T_K (K)
UAl_2	≈ 50	≈ 100	820	91	0.11	0.27	6	270
$CeSi_{1.85}$	≈ 100	≈ 140	410	120	0.29	0.37	13	140
UPt_3	≈ 150	≈ 270	270	95	0.35	0.46	15	90

is suppressed at low temperatures much below T_{SF}. In particular, the suppression is almost perfect in alloyed compounds such as $UPt_{3-x}Pd_x$ (Ref. 39) and $UAl_{2-x}Pr_x$.[19] It has already been pointed out that impurities suppress the logarithmic term.[40]

The fitted parameters listed in Table I depend on fitted regions of temperatures. When data are fitted at lower temperatures and as long as the logarithmic term is observed, the fitted δ is higher, while the fitted T_{SF} is lower for UAl_2.[19] This tendency implies that the suppressions of the logarithmic term by impurities appears before low enough temperatures are reached for the asymptotic expression. If the temperature regions are restricted to a narrow region, even the theoretical results in Figs. 1 and 2 can be approximately fitted by another logarithmic dependence with slightly different parameters even above $T > 0.3T_{SF}$. The main origin of a small difference between fitted and theoretical T_{SF} is presumably due to the fitted region of temperatures, whose lower limit is presumably restricted by the suppression due to impurities.

In the present theory, $J_{RKKY}(0,0)$ is approximately scaled with T_K. Therefore, it can be expected that one-parameter scaling[35,36] should be approximately satisfied even in paramagnon effects. It is interesting to examine experimentally paramagnons under pressures, which can make T_K high.

It is likely that $J_{RKKY}(0,0)$ is positive in many heavy-electron compounds. Therefore, it is likely that paramagnons also play roles in many heavy-electron compounds. However, no observations of the logarithmic term have been reported for typical Kondo lattices with very low local Kondo temperatures of the order of $T_K \approx 10$ K. This is reasonable, because low local Kondo temperatures imply much lower spin-fluctuation temperatures T_{SF} of paramagnons. A simple scaling of energy scales gives $T_{SF} \approx 0.2$ K for $T_K \approx 10$ K. It is interesting to examine experimentally the specific heat below 0.1 K of very clean typical Kondo lattices such as $CeCu_6$.

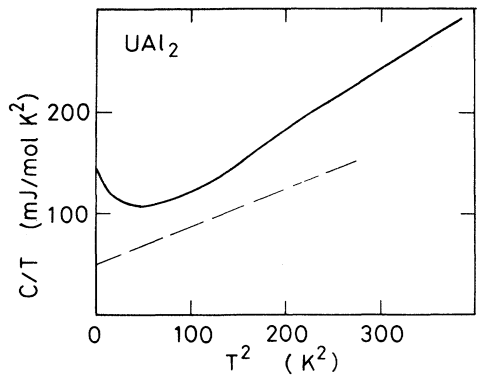

FIG. 5. Specific heat C/T of UAl_2 as a function of T^2. The solid line is an experimental result of Ref. 19, and the dashed line is assumed to be due to local spin fluctuations and phonons $\gamma_{loc}+\beta T^2$, with $\beta = 0.2$ mJ/(mol K^4) from Ref. 19.

Actually, $CeSi_{2-x}$ shows ferromagnetism for $x > 0.17$. Therefore, it is certain that paramagnons are responsible for the low-temperature specific heat of $CeSi_{2-x}$. Because estimated numbers of the cutoff ($q_c/2k_F$) are not small for UAl_2, $CeSi_{1.85}$, and UPt_3, ferromagnetic spin fluctuations of paramagnons should be rather extended in the Brillouin zone. It is interesting to observe directly such ferromagnetic spin fluctuations by neutron scattering, although their characteristic energy is as small as $k_B T_{SF} \approx 1$ meV.

The resistivity due to local spin fluctuations obeys the T^2 law much below T_K, it has a peak around T_K, and it obeys the well-known logarithmic law above T_K. Because the backward scatterings have the main contribution to the resistivity, the effects of paramagnons are small for the resistivity. On the other hand, the effects of antiferromagnetic fluctuations can be large, even if they are only developed in a narrow region of the Brillouin zone. If their energy scale T_a is as small as T_K, the resistivity at low temperatures should be mainly due to antiferromagnetic spin fluctuations. In such cases, therefore, it is presumably difficult to observe the well-known logarithmic dependence in the raw data of resistivity. It is likely that the resistivity of UPt_3 is mainly due to antiferromagnetic spin fluctuations, because such spin fluctuations have actually been observed by neutron scattering.[3,4]

Konno and Moriya[38] have recently argued that the logarithmic term due to paramagnons can only be observed at extremely low temperatures such as $T \ll T^*$ with $T^* \approx A^{1/2}T_p$ in the notation of this paper. They estimated as $T^* = 0.20$–16.9 K for $A = 0.01$–0.1 in case of UAl_2 and $T^* = 0.07$–17.7 K for $A = 0.01$–2.0 in case of UPt_3. From Fig. 2 in Ref. 37, T_{SF} is estimated as $T_{SF} \approx 0.1T^*$ or 0.02–2 K. Therefore, they concluded that the observed logarithmic term is unlikely to be due to paramagnons, because it can be only observed below T_{SF}. However, once T_{SF} is given, the asymptotic expression can also be used in $T < 0.3T_{SF}$ even in their analysis, as can be seen from, for example, Fig. 2 in Ref. 38 and

Figs. 1 and 2 in this paper. Therefore, if experimental numbers of $T_{SF} \approx 10$ K are used, it seems to be difficult to conclude that the effects of paramagnons are enough small to be ignored below 10 K.

They argued in a phenomenological theory that the specific heat due to "localized paramagnons" can simulate approximately Eq. (1.1) including the logarithmic term in an intermediate temperature region. However, their localized paramagnons must be different from local spin fluctuations in the SSA. If T_K is much higher than 10 K, the specific heat should be in proportion to T below 10 K. If T_K is about 10 K, on the other hand, the linear specific-heat coefficient should be as large as 1 J/(mol K^2). In any event, local spin fluctuations in the SSA cannot simulate the observed logarithmic temperature dependence of the specific heat.

V. DISCUSSION

It can be naively argued that results are only applicable to high-energy phenomena in a crude approximation of nonvariational methods and the results become applicable even to low-energy phenomena in a higher approximation. The naive argument holds in the present theory. It is straightforward to see that if the simplest single-site diagrams of $K_\sigma(i\varepsilon)$ are included in the present auxiliary-particle method, two broad peaks are reproduced far from the chemical potential around ε_f and $\varepsilon_f + U$ in the density of states of f electrons.[41] In the best SSA, on the other hand, not only such broad peaks, but also the heavy-electron band at the chemical potential is obtained as examined in Sec. II. Therefore, the present theory can deal with both high- and low-energy phenomena.

On the other hand, the mean-field or saddle-point approximation of auxiliary particles,[11–13] which is one of the simplest approximations, certainly gives a heavy-electron band similar to the heavy-electron band obtained in the Gutzwiller approximation and the best SSA. However, any mean-field theories or their extensions have never reproduced the broadbands far from the chemical potential so far. Because variational methods concern with the ground state, it is reasonable that the Gutzwiller approximation can only deal with low-energy phenomena. However, it is unusual that a lowest approximation of the nonvariational method can only deal with low-energy phenomena. Because charge fluctuations are relevant for high-energy phenomena in strongly correlated systems in general, the description of charge fluctuations at high energies is totally incorrect in the mean-field approximation.

Even if we are concerned with low-lying fluctuations, the difference is also essential in charge fluctuations. There are a lot of low-lying charge fluctuations in the mean-field approximation (MFA), where the accumulation of charge fluctuations at low energies is consistent with the absence of charge fluctuations at high energies. However, the suppression of low-lying charge fluctuations is likely in strongly correlated systems. Low-lying charge fluctuations are actually much suppressed in the present theory.

The mean-field approximation assumes that the local gauge symmetry is broken. The physical consequence of this approximation is that unphysical properties such as $\langle a_{i\sigma}^\dagger a_{j\sigma} \rangle$, $\langle e_i^\dagger e_j \rangle$, and $\langle d_j^\dagger d_j \rangle$ with $i \neq j$ are finite, which are not in the gauge-invariant form. Therefore, auxiliary particles are itinerant, and narrow bands of auxiliary particles are formed at their chemical potentials. Itinerant a particles are nothing but spinons, and itinerant e particles are nothing but holons in the MFA of the resonating valence-bond (RVB) theory.[42] In general, charge fluctuations are essentially related with itinerancy of particles. Therefore, the accumulation of low-lying charge fluctuations is due to the itinerancy of auxiliary particles. Because of itinerancy, spin and charge fluctuations are almost equivalent in the mean-field approximation. Although the expectation value of the unphysical properties can be made to vanish by including fluctuations of gauge fields, their low-lying excitations associated with the gauge fields are still essentially responsible for low-lying spin and charge fluctuations beyond the mean-field approximation.

The local gauge symmetry should never be broken in order to guarantee the mapping between the real- and auxiliary-particle models. Because either $\langle a_{i\sigma}^\dagger a_{j\sigma} \rangle$ with $i \neq j$, $\langle e_j^\dagger e_j \rangle$ with $i \neq j$, or $\langle d_i^\dagger d_j \rangle$ with $i \neq j$ does not conserve the local number of auxiliary particles either Q_i and Q_j, it is quite trivial that they should vanish unless the local gauge symmetry is broken. Auxiliary particles should be localized in the sense that their single-particle Green functions are site diagonal. Because of infinitely large repulsion U_∞ between auxiliary particles, an excitation energy as large as U_∞ is required to add an auxiliary particle or to remove an auxiliary particle within the restricted Hilbert space. It means that auxiliary particles are confined in low-energy phenomena in the sense that no single-particle excitations are possible. Because of the localization and confinement, auxiliary fermions have no Fermi surfaces or auxiliary bosons never show any Bose condensation.[41]

It is obvious that as long as the mapping is rigorously taken into account, the local gauge symmetry should never be broken in any approximations of auxiliary-particle methods, and the localization and confinement should also not be broken. Therefore, the present theory is totally different from the mean-field approximation and any of its extensions, because the two schemes are developed in totally different Hilbert spaces. Although low-lying spin fluctuations are similar, there is no correspondence between the two schemes.

IV. SUMMARY

A theory of almost localized magnetism is applied to paramagnons in heavy-electron compounds. There are three relevant parameters. One is the local Kondo temperature T_K or the renormalized Fermi energy $T_F^* \approx 3T_K$. Another is the enhancement factor of the homogeneous susceptibility $1/A$. The other is the cutoff of paramagnons in the momentum space, $y_c = q_c/2k_F$, with k_F the Fermi wave vector. The specific-heat coefficient due to local spin fluctuations is proportional to $1/T_F^*$. The linear specific-heat coefficient due to paramagnons is pro-

portional to y_c^2/T_p, with $T_p = AT_F^*$. The logarithmic $T^3 \ln T$ term of the specific heat is proportional to T_p^{-3}, which can be observed below $T_{SF} = \theta A^{1/2} T_p$ with $\theta < 1$. The constant θ depends on both A and y_c. For example, θ is much smaller than unity if the enhancement factor $1/A$ is large and/or if paramagnons are sharply localized in the Brillouin zone. However, θ is about 0.2, unless $1/A$ is very large and unless the spin fluctuations are much confined.

The specific heats of UAl_2, $CeSi_{1.85}$, and UPt_3 are analyzed. Both local spin fluctuations and paramagnons must contribute to the specific heat at low temperatures. It is very likely that the logarithmic terms at low temperatures $T < 10$ K are due to paramagnons.

Note added in proof. Momentum conservation is not essential in the $d = +\infty$ dimension as argued in W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989); E. Müller-Hartman, Z. Phys. B **74**, 507 (1989); H. Schweitzner and G. Czycholl, Solid State Commun. **69**, 171 (1989); and U. Brandt and C. Mielsh, Z. Phys. B **75**, 365 (1989). Almost all the leading-order terms with respect to $1/d$ are included in the best SSA. The other leading-order effect is a MFA type of magnetism, as exclaimed in the Hubbard model in Ref. 30. The situation is the same even in the periodic Anderson model. Therefore the perturbative scheme from the best SSA in this paper is nothing but the $1/d$ expansion from the $d = +\infty$ dimension.

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