# Mechanism for heavy-fermion superconductivity

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A method has been developed to obtain an effective interaction between heavy quasiparticles that exist in heavy-fermion systems by combining the effects of the Coulomb interactions and the electron-phonon interactions that act among various constituents (heavy quasiparticles, light quasiparticles, phonons, non- $f$  atoms) of the system. The effective interaction is expressed in terms of microscopic parameters of the heavy-fermion systems. The role of the new effective interaction in determining superconducting order in heavy-fermion systems at low temperatures has been clarified. It is found that an appropriate strength of the new interaction leads to  $p$ -wave superconductivity. Values of the superconducting transition temperature calculated by using the new interaction for different heavy-fermion systems are in good agreement with the experimental values of the superconducting transition temperature for reasonable magnitudes of quasiparticle bandwidths. General features of the new interaction have been discussed.

#### I. INTRODUCTION

Heavy-fermion systems are those intermetallic compounds in which the effective mass of conduction electrons, as obtained from the specific-heat values, is typicaltrons, as obtained from the specific-heat values, is typically 10 to 100 times the bare electron mass.<sup>1,2</sup> One of the metallic constituents of these compounds is made of such  $f$  atoms which have partially filled  $f$  orbitals (Ce,U,Np), while the other metallic constituent(s) is (are) made of non-f atoms. In most of the heavy-fermion systems (except for, e.g.,  $CePb_3$ ) the f atoms are heavier than the non-f atoms. For specificity we shall consider only such heavy-fermion systems in which f atoms are heavier. However, the present formalism can be suitably generalized to the other type of the heavy-fermion systems, also.

Non-f atoms play three major roles in heavy-fermion systems: (i) Non- $f$  atoms play a role in the determination of crystal structures of the heavy-fermion systems. (ii) Non- $f$  atoms increase the distance between  $f$  atoms. This results in reduction of direct interactions between the  $f$  atoms so that their  $f$  electrons will move mainly in the atomiclike  $f$  states. On the other hand, due to large spatial extensions, the  $d$  electrons of the  $f$  atoms will move in band states. (iii) Electrons of the non-f atoms will interact with the  $f$  and  $d$  electrons of  $f$  atoms, and will affect the properties of the system. Due to smaller mass, the vibrational amplitudes of non-f atoms will generally be larger than that of  $f$  atoms. Because of these large vibrational amplitudes the interactions between electrons from non- $f$  atoms and  $f$  and  $d$  electrons will be enhanced. This aspect has not so far been considered in heavy-fermion systems, although a similar role of non-f atoms has been considered in other intermetallic systems.

Apart from the interaction effects of the non-f atoms on the  $f$  and  $d$  electrons, there are many other interactions which exist in heavy-fermion systems. Important among them are hybridization interaction between  $f$  and  $d$  electrons; spin-orbit interaction in  $f$  atoms; crystal field; on-site Coulomb interaction between  $f$  electrons; Coulomb interaction between  $f$  and  $d$  electrons; electron-phonon interaction; and anharmonic interaction<br>A number of methods<sup>2,4–11</sup> have been developed to trea these interactions for studying different properties (magnetic, superconducting, etc.) of heavy fermion systems in various temperature regimes. For the particular case of the superconducting order which appears at low temperatures in some of the heavy-fermion systems, the main methods for treating the above interactions are as follows. A number of workers have used group-theoretical methods<sup>2,4</sup> for treating the effects of the crystal field and/or spin-orbit interaction without considering other interactions. Such methods are useful only for the study of the symmetry properties of the superconducting order parameter. There is no clarification of the interaction mechanism of superconductivity in these methods. Many workers<sup>2,4,5</sup> have treated the effect of electronic interactions through such effects as the Kondo volume collapse effect<sup>2</sup> or the magnetoelastic effect<sup>12</sup> by considering the electron-phonon interaction as the source of heavyfermion superconductivity. In many other treatments of various interactions<sup>2,4</sup> the electron-phonon interaction is neglected while electronic interactions are treated within the frameworks of the Fermi liquid theory,<sup>2,6</sup> Kondo boson theory,<sup>2</sup> Hubbard model,<sup>2,8</sup> and other perturbative or variational methods.<sup>2,7</sup> Fay and Appel<sup>9</sup> and Kim<sup>10</sup> have considered the effect of electron-phonon interaction also along with the treatment of electronic interactions. Jichu along with the treatment of electronic interactions. Jich<br>et al.<sup>11</sup> have treated the electronic and electron-phono interactions separately and have found two alternative sources of superconductivity—one based on electronic interactions, the other based on electron-phonon interaction through Kondo volume collapse.

Different methods, mentioned above, lead to different predictions regarding the nature of superconductivity in heavy-fermion systems. Some of them, based mainly on phonon-mediated interactions, predict s-wave superconductivity, while others, based mainly on electronic in-

teractions, predict  $p$ -wave or  $d$ -wave superconductivity. teractions, predict p-wave or d-wave superconductivity<br>In the absence of any experimental evidence,<sup>1,13</sup> it is not possible to say which prediction is correct.

Most of the methods mentioned above have tenuous relevance to heavy-fermion systems in that these are based on ideas borrowed<sup>4</sup> from conventional superconductors, superfluid  ${}^{3}$ He, Hubbard model, and Kondo bosons. We have put forward here an approach which treats the interactions which exist in heavy-fermion systems in such a manner that their effects finally appear through microscopic parameters of the system (like lattice constant, masses of  $f$  atoms and non- $f$  atoms, and number of non- $f$  atoms per  $f$  atom). The interactions considered in the present study are described in Sec. II. In Sec. III the new method for treating the interactions is described, and an effective interaction is obtained between heavy quasiparticles. In Sec. IV we describe how the new effective interaction between heavy quasiparticles combines with the Coulomb interaction between heavy quasiparticles to determine the superconducting order in heavy-fermion systems at low temperatures. Results of our calculations of superconducting transition temperature for a number of heavy-fermion systems have been presented in Sec. V. In Sec. VI, we draw conclusions regarding the present method.

# II. HAMILTONIAN OF HEAVY-FERMION SYSTEMS

We assume that the " $nf$ " electrons interact with the " $(n + 1)d$ " band electrons only, and not with the " $(n+2)s$ " band electrons (n = 4 for Ce-based systems, while  $n = 5$  for U- and Np-based systems), so that the role of the " $(n + 2)s$ " band electrons is only to contribute to the screening of various interactions which exist in the heavy-fermion systems. Coupling of the  $f$  electrons with the d band electrons is characterized by the Anderson hybridization interaction  $V$  which leads to formation of two quasiparticle bands—the lower one of which will have mainly f character, while the upper one will have mainly d character. One of the effects of quasiparticle band formation will be that the  $f$  state will assume an energy width of order  $\Delta_F \sim \pi \rho_F V^2$ , where  $\rho_F$  is the density of states at the Fermi energy  $E_F$ . When this energy width  $\Delta_F$  is much smaller than the magnitude of the f state energy  $E_f$  ( $\Delta_F \ll |E_f|$ ), and when  $E_f$  lies below  $E_F$ , then near to the Fermi wave vector the lower quasiparticle band will be flat,  $14, 15$  while the upper one will not be so. Consequently, a lower band quasiparticle will have much larger effective mass,  $m_1^* \gg m$ , while the mass of the upper band quasiparticle will be similar to the bare mass of an election,  $m_2^* \sim m$ . Here,  $m_\alpha^*$  is the effective mass of an electron in the  $\alpha$ th quasiparticle band ( $\alpha$ =1 for the lower band,  $\alpha = 2$  for the upper band).

The process of hybridization of the atomiclike  $f$  states with the delocalized  $d$  states in heavy-fermion systems is described by the Anderson lattice Hamiltonian which, in terms of quasiparticle operators, can be written as

$$
H_A = \sum_{\alpha \mathbf{k} s} E_{\alpha}(\mathbf{k}) \gamma_{\alpha s}^{\dagger}(\mathbf{k}) \gamma_{\alpha s}(\mathbf{k}) . \tag{1}
$$

Here,  $\gamma_{\alpha s}^{\dagger}(\mathbf{k})$  and  $\gamma_{\alpha s}(\mathbf{k})$  denote, respectively, the

creation and annihilation operators of the quasiparticles in the  $\alpha$ th band with spin s, wave vector k, and energy  $E_{\alpha}(\mathbf{k})$  such that when  $V\rightarrow 0$ , then  $\gamma_{1s}(\mathbf{k})\rightarrow f_{s}(\mathbf{k}),$  $\gamma_{2s}^{\alpha}(\mathbf{k}) \rightarrow d_s(\mathbf{k}), E_1(\mathbf{k}) \rightarrow E_f$ , and  $E_2(\mathbf{k}) \rightarrow E_d(\mathbf{k}).$   $f_s^{\dagger}(\mathbf{k})$ and  $f_s(\mathbf{k})$  are creation and annihilation operators of an electron in the dispersionless f band;  $d_s^{\dagger}(\mathbf{k})$  and  $d_s(\mathbf{k})$  are corresponding operators of an electron in the d band.  $E_d(\mathbf{k})$  is the energy of an electron in the d band states of wave vector **k**.

Notice that for nonzero  $V$  the quasiparticle energies  $E_{\alpha}(\mathbf{k})$  will be complex,<sup>16</sup> although in the framework of the Fermi liquid theory the wave vector k will be real. In this paper we avoid working with complex energies and treat  $E_{\alpha}(\mathbf{k})$  to be real quantities in which the effect of V is included through the quasiparticle bandwidths  $W^*_{\alpha}$ . Since  $m_1^* \gg m$  and  $m_2^* \sim m$ , we use (nearest-neighbor) tight-binding approximation for the lower band, and free particle approximation for the upper band. In this sense the energies  $E_{\alpha}(\mathbf{k})$  can be written as

$$
E_1(\mathbf{k}) = E_f - (W_1^* / z) \sum_i^{(NN)} \exp(i\mathbf{k} \cdot \mathbf{R}_i) - E_F
$$
 (2)

and

$$
E_2(\mathbf{k}) = E_2(\mathbf{o}) + \hbar^2 k^2 / 2m_2^* - E_F
$$
 (3)

Here, z is coordination number,  $\mathbf{R}_i$  is direct lattice vector at lattice equilibrium, and  $\hslash$  is the Plank's constant divided by  $2\pi$ . The superscript (NN) on the summation denotes that the sum is over nearest-neighbor sites only. Typical values of the lower quasiparticle bandwidth  $W_1^*$ Typical values of the lower quasiparticle bandwidth  $W_1^*$ <br>are 2 meV for Ce-based systems,  $^{17,18}$  and 4–6 meV for Ubased systems.<sup>17,18</sup>

Since the lower band quasiparticles are heavier we call them heavy quasiparticles, while we call the upper band quasiparticles light quasiparticles. We introduce various interactions among these quasiparticles. First of all we consider the on-site (screened) Coulomb interaction between  $f$  electrons,  $U$ . During the process of quasiparticle formation, U will be renormalized by the hybridization interaction  $V$ , and will act among all the (heavy as well as light) quasiparticles in a complicated manner. In fact there will be a number of interaction terms among quasiparticles due to U. But as has been argued by Cyrot,<sup>8</sup> only two of them will be important. These terms are

$$
H_U = U \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \gamma_{11}^\dagger(\mathbf{k}+\mathbf{q})\gamma_{11}^\dagger(\mathbf{k}'-\mathbf{q})\gamma_{11}(\mathbf{k}')\gamma_{11}(\mathbf{k}) \tag{4}
$$

and

$$
H_K = J_K \mathbf{S}_1 \cdot \mathbf{S}_2 \tag{5}
$$

Here, the V- and U-dependent interaction  $J_K$  is a Kondo-like interaction; and  $S_{\alpha}$  is the spin operator of the  $\alpha$ th band quasiparticle. We follow Cyrot, and neglect other contributions of U.

We now consider a (screened) Coulomb interaction,  $U_{fd}$ , between an f electron and a d electron. Like the interaction U,  $U_{td}$  will also lead to a number of interaction terms between the heavy quasiparticles, light quasiparticles, and heavy and light quasiparticles. Just like the most significant effect of  $U$  occurs as a two-body interaction between heavy quasiparticles, Eq. (4), the most significant effect of  $U_{fd}$  will be between a heavy quasiparticle and a light quasiparticle. The effect of  $U_{fd}$  between heavy quasiparticles will be much smaller than  $U$ , and so it can be neglected. The effect of  $U_{fd}$  between light quasiparticles will also be negligibly small. So, we approximate the effect of  $U_{fd}$  among various quasiparticles by a two-body interaction between a heavy quasiparticle and a light quasiparticle—we denote this interaction by  $W_c(\mathbf{r}_{1i} - \mathbf{r}_{2i})$  in the coordinate representation, and by  $V_c(q)$  in the momentum representation. Here,  $r_{ai}$  is the position coordinate of the *i*th  $\alpha$  quasiparticle and **q** is momentum transfer.

Before saying anything regarding the form of, say,  $W_C(\mathbf{r}_{1i} - \mathbf{r}_{2i})$ , let us have a look at the form of  $J_K$  which also acts between a heavy quasiparticle and a light quasiparticle.  $J_K$  depends explicitly on V and U (see above). We have taken  $V$  as a constant interaction for a given heavy-fermion system. In order to keep the form of  $J_K$ consistent, we must consider  $U$  also as a constant interaction. However, we can accommodate in our formulation a more realistic form of  $W_C(\mathbf{r}_{1i} - \mathbf{r}_{2i})$ , rather than taking it a constant interaction by specifying it  $(W<sub>C</sub>)$  as a (screened) Coulomb interaction between a heavy quasiparticle and a light quasiparticle. We can, therefore, write  $W_C(\mathbf{r}_{1i} - \mathbf{r}_{2i})$  as follows:

$$
W_C(\mathbf{r}_{1i} - \mathbf{r}_{2j}) = e^2 \exp(-\lambda_C |\mathbf{r}_{1i} - \mathbf{r}_{2j}|)/|\mathbf{r}_{1i} - \mathbf{r}_{2j}|.
$$
 (6)

Here, e is the electric charge of an electron and  $1/\lambda_c$  is the screening length.

The Fourier transform of  $W_C(\mathbf{r}_{1i} - \mathbf{r}_{2i})$  is given by

$$
V_C(\mathbf{q}) = 4\pi e^2 / q^2 \Omega \epsilon(\mathbf{q}) \tag{7}
$$

Here,  $\Omega$  is unit cell volume, and  $\epsilon(q)=1 + \lambda_C^2/q^2$  is a static screening function caused by " $(n+1)d$ " and " $(n+2)s$ " electrons. The contribution of the screened Coulomb interaction to the Hamiltonian of the system is

$$
H_C = 2^{-1} \sum_{i,j} W_C(\mathbf{r}_{1i} - \mathbf{r}_{2j}) \tag{8}
$$

We now consider the quasiparticle-phonon interaction. Different types of methods based on, e.g., Kondo volum collapse<sup>2,4,11</sup> and deformation potential<sup>4,5</sup> have alread been developed to calculate this interaction. Here we consider the quasiparticle-phonon interaction in its most elementary form,<sup>19</sup>

$$
\tilde{V}(\mathbf{r}_{\alpha i}) = \sum_{j} \mathbf{Q}_{j} \cdot \nabla V_{ei}(\mathbf{r}_{\alpha i} - \mathbf{R}_{j}) \tag{9}
$$

Here,  $Q_i$  is the displacement of jth ion of the lattice from the lattice equilibrium  $\mathbf{R}_j$ ; and  $V_{ei}(\mathbf{r}_{ai} - \mathbf{R}_j)$  is a screened electron-atom potential

$$
V_{ei}(\mathbf{r}_{\alpha i} - \mathbf{R}_j) = Ze^2 \exp(-\lambda_C |\mathbf{r}_{\alpha i} - \mathbf{R}_j|)/|\mathbf{r}_{\alpha i} - \mathbf{R}_j|.
$$
\n(10)

Here,  $-Ze$  is the charge of an atomic ion.

The contribution of  $\tilde{V}(\mathbf{r}_{\alpha i})$  to the Hamiltonian of the system is given by

$$
H_{\text{qp-ph}} = \sum_{\alpha \mathbf{k} \mathbf{q} s j} M_j^{(\alpha)}(\mathbf{q}) \gamma_{\alpha s}^{\dagger}(\mathbf{k} + \mathbf{q})
$$
  
 
$$
\times \gamma_{\alpha s}(\mathbf{k}) [b_j^{\dagger}(-\mathbf{q}) + b_j(\mathbf{q})]. \tag{11}
$$

Here,

$$
M_j^{(\alpha)}(\mathbf{q}) = -V_{ei}^{(\alpha)}(\mathbf{q})\mathbf{q}\cdot\hat{\boldsymbol{\xi}}_j(\mathbf{q})[\boldsymbol{\hbar}/2M_fNw_j(\mathbf{q})]^{1/2} ,\qquad (12)
$$

with  $V_{ei}^{(\alpha)}(q)$  as the Fourier transform of  $V_{ei}(\mathbf{r}_{\alpha i} - \mathbf{R}_j)$ ,  $\hat{\xi}_i(q)$  as the polarization vector of phonons,  $M_f$  as the mass of an  $f$  atom,  $N$  as the number of ions in the solid, and  $w_i(q)$  as the frequency of a phonon in the *j*th branch. The phonon Hamiltonian is given by

$$
H_{\rm ph} = \sum_{j\mathbf{q}} \hbar w_j(\mathbf{q}) b_j^{\dagger}(\mathbf{q}) b_j(\mathbf{q}) . \qquad (13)
$$

Finally, we introduce the effect of large vibrations of non-f atoms on the quasiparticles. Let this effect be denoted by the interaction  $V_{nf}$ . We shall treat the effect of  $V_{nf}$  phenomenologically in the next section. Here, we just include this interaction in the Hamiltonian of the system through the interaction operator  $H_{nf}$ .

Summing all the interaction operators considered above we can write down a Hamiltonian of heavyfermion systems as follows:

$$
H = H_A + H_U + H_K + H_C + H_{\text{qp-ph}} + H_{nf} + H_{\text{ph}} \tag{14}
$$

From the viewpoint of the interaction mechanism of superconductivity this Hamiltonian contains much more details of interactions than those considered by other workers.<sup>2,4</sup> Crystal field and spin-orbit interaction are not included in  $H$  for practical reasons.

#### III. TREATMENT OF INTERACTIONS

Experimental data on the specific-heat jump show that superconductivity in heavy-fermion systems is due to heavy quasiparticles.<sup>1</sup> We therefore combine all the interaction effects which are involved in  $H$  to obtain an effective interaction between heavy quasiparticles. As we have mentioned in Sec. I, a number of methods based on Fermi liquid description, perturbation techniques, and variation techniques have already been developed to treat various interactions in heavy-fermion systems. In this paper, we employ a perturbation method to obtain an effective interaction between heavy quasiparticles. Roughly speaking, our method is similar to the well<br>known RKKY (Ruderman-Kittel-Kasuya-Yosida) known RKKY (Ruderman-Kittel-Kasuya- Yosida) method, $20$  but we have included more interactions than in the RKKY method. The main steps of our perturbation method are as follows. First of all, we consider the phonon-mediated interaction between heavy quasipartieles. Then, we consider a phonon-mediated interaction between heavy and light quasiparticles, which we denote in the coordinate representation by  $W_{ph}(\mathbf{r}_{1i} - \mathbf{r}_{2i})$ . We combine this interaction with the screened Coulomb interaction  $W_C(\mathbf{r}_{1i} - \mathbf{r}_{2i})$ , in a manner used earlier in heavily doped semiconductors.<sup>21</sup> We denote the combined interaction by  $W(\mathbf{r}_{1i} - \mathbf{r}_{2j})$ , i.e.,  $W(\mathbf{r}_{1i} - \mathbf{r}_{2j}) = W_C(\mathbf{r}_{1i})$  $(\mathbf{r}_{2j})+W_{\text{ph}}(\mathbf{r}_{1i}-\mathbf{r}_{2j}).$  From  $W(\mathbf{r}_{1i}-\mathbf{r}_{2j})$  we obtain direct and exchange interactions between heavy and light quasiparticles. Let the most effective part of the resultant of direct and exchange interactions (see below) be denoted by  $J^{(12)}(q)\sigma^{(1)}\sigma^{(2)}$ , where  $J^{(12)}(q)$  is the exchange integral for the wave vector transfer q, and  $\sigma^{(\alpha)}$  is the Paul spin operator for the  $\alpha$ th quasiparticle. This interaction has the same nature as that of  $J_K S_1 \cdot S_2$ , Eq. (5). So we combine  $J^{(12)}(q)$  and  $J_K$  to obtain  $\tilde{J}^{(12)}(q) = J^{(12)}(q) + J_K$ . In order to obtain an effective interaction between heavy quasiparticles from  $\tilde{J}^{(12)}(q)$ , we proceed in a manner similar to that of the RKKY method. This leads us to the following form of the effective interaction between heavy quasiparticles.

$$
H_{11} = \sum_{\substack{\mathbf{k}\mathbf{k}'\mathbf{q} \\ ss's's''s'''}} J^{(11)}(\mathbf{q})\sigma_{ss'''}^{(1)}\cdot\sigma_{s's''}^{(1)}\cdot\gamma_{1s''}^{\dagger}(\mathbf{k}+\mathbf{q})
$$
  
 
$$
\times \gamma_{1s''}^{\dagger}(\mathbf{k}'-\mathbf{q})\gamma_{1s'}(\mathbf{k}')\gamma_{1s}(\mathbf{k}) . \qquad (15)
$$

Here,

$$
J^{(11)}(q) = [\tilde{J}^{(12)}(q)]^2 P(q) , \qquad (16)
$$

with  $P(q)$  as the polarization function of the light quasiparticles. This approximation will be justified only when the characteristic energy corresponding to  $\tilde{J}^{(1\tilde{2})}(\mathbf{q})$  is much smaller than the characteristic energy corresponding to  $J^{(11)}(q)$ . The characteristic energy corresponding to  $\widetilde{J}^{(12)}(q)$  is

$$
\widetilde{E}^{(12)} \sim W_2^* \exp[-1/\widetilde{J}^{(12)}({\bf k}_F)\rho_{2F}^*],
$$

where  $\mathbf{k}_F$  is the Fermi wave vector, and  $\rho_{2F}^*$  $=\Omega m_z^* k_F / \pi^2 \hbar^2$  is the density of upper quasiparticle band states at the Fermi energy. The characteristic energy corresponding to  $J^{(11)}(q)$  is

$$
E^{(11)} \sim (\tilde{J}^{(12)})^2 / W_2^*
$$

Thus the approximation of Eqs. (15) and (16) will be Thus the approximation of Eqs. (15) and (16) will b justified if  $\tilde{E}^{(12)} \ll E^{(11)}$ . If this condition is not satisfied justified if  $E^{(12)} \ll E^{(11)}$ . If this condition is not satisfied there will be a need for considering  $\tilde{J}^{(12)}(q)$  beyond second order. We do not consider  $\tilde{J}^{(12)}(q)$  beyond second order for reasons of simplicity.

Until now we have not said anything regarding the interaction  $V_{nf}$  which was introduced in H, Eq. (14), through  $H_{nf}$ . In order to incorporate an effect of  $V_{nf}$ , we realize that the polarization function  $P(q)$ , Eq. (16), orig-<br>inates from the mediation of the effect of the interaction  $\tilde{J}^{(12)}(q)$  by light quasiparticles. While mediating the effect of  $\tilde{J}^{(12)}(q)$  the light quasiparticles will feel the effect of large vibrational amplitudes of non-f atoms. The vibrational amplitude of a non- $f$  atom is about twice the vibrational amplitude of an  $f$  atom. This indicates that there will be a significant effect of  $V_{nf}$  on the polarization of the medium of light quasiparticles. For simplicity, we assume that the effects of  $\tilde{J}^{(12)}(q)$  and  $V_{nf}$  on the light quasiparticles act independently so that we can write the polarization operator  $P(q)$  in the following factor form:

$$
P(\mathbf{q}) = P_0(\mathbf{q}) P_{nf} \tag{17}
$$

Here  $P_0(q)$  is the polarization operator with  $V_{nf}=0$ . The effect of nonzero value of  $V_{nf}$  is taken care of by the factor  $P_{nf}$ .  $P_0(q)$  is given by its usual expression,<sup>22</sup> and a form of  $\tilde{P}_{nf}$  is obtained below.

### A. Phonon-mediated interaction between heavy quasiparticles

The speed of heavy quasiparticles is quite slow, about 100 times less than that of light quasiparticles. So, when a region of lattice is polarized by a heavy quasiparticle, another heavy quasiparticle will take a long time to reach this polarized region and the polarization may decay by that time. For this reason the interaction mediated by phonons between two heavy quasiparticles will be negligibly small. We therefore will not consider this interaction. It must, however, be noted that in other methods<sup>2</sup> which use phonon-mediated interaction as a driving mechanism for superconducting order, phonon-mediated interactions between heavy quasiparticles come out to be significant because in these methods effects like Kondo volume collapse which are based on electronic interactions are used. In the present method we treat the electronic interactions on the same footing as for the quasiparticle-phonon interaction.

## B. Phonon-mediated interaction between heavy and light quasiparticles

Suppose a region of lattice is polarized by a heavy quasiparticle. Then, due to its fast speed a light quasiparticle can reach this region before the polarization of this region can decay significantly. This means that the phonon-mediated interaction between heavy and light quasiparticles will achieve significance, and must be considered along with other interactions. We can express the phonon-mediated interaction between heavy and light quasiparticles as follows:

$$
W_{\text{ph}}(\mathbf{r}_{1i} - \mathbf{r}_{2j}) = \sum_{\mathbf{q}} V_{\text{ph}}(\mathbf{q}) \exp[i\mathbf{q} \cdot (\mathbf{r}_{1i} - \mathbf{r}_{2j})] \ . \tag{18}
$$

Here,

$$
V_{\text{ph}}(\mathbf{q}) = \sum_{j} |M_j^{(1)*}(\mathbf{q})M_j^{(2)}(\mathbf{q})|D_j(\mathbf{q}) , \qquad (19)
$$

with  $D_i(q) = -2/w_i(q)$  as the phonon Green function at zero frequency. In Eq.  $(19)$  we have neglected retardation effects for two reasons. The first reason for the neglect of retardation effects in the phonon-mediated interaction is that it is necessary for a consistent addition of  $W_{\rm ph}$  and  $W_C$ , Eq. (6), because we have not considered retardation effects in  $W_C$ . Secondly, the neglect of retardation effects renders expressions of relevant quantities (transition temperature, etc.) amenable to practical calculations.

# C.  $J^{(12)}(q)$  from  $W(r_{1i} - r_{2i})$

The combined interaction  $W(\mathbf{r}_{1i} - \mathbf{r}_{2i})$  will lead to a direct interaction, say  $K^{(12)}(q)$ , and an exchange interaction, say  $E_{\text{ex}}^{(12)}(\mathbf{q})$ , between heavy and light quasiparticle It is well known<sup>23</sup> that a part of  $E_{\text{ex}}^{(12)}(\mathbf{q})$  suppresses the effect of  $K^{(12)}(q)$  almost completely so that we need to consider only the remaining part of  $E_{\text{ex}}^{(12)}(\mathbf{q})$ . We identify<br>the remaining part of  $E_{\text{ex}}^{(12)}(\mathbf{q})$  as  $J^{(12)}(\mathbf{q})\mathbf{S}_1 \cdot \mathbf{S}_2$ . This the remaining part of  $E_{\text{ex}}^{(q)}(q)$  as  $J^{(r)}(q)$  means that we can express  $J^{(12)}(q)$  as follows

$$
J^{(12)}(\mathbf{q}) = \int \psi_2^*(\mathbf{k}_2 + \mathbf{q}, \mathbf{r}_{1i}) \psi_1^*(\mathbf{k}_1 - \mathbf{q}, \mathbf{r}_{2j}) W(\mathbf{r}_{1i} - \mathbf{r}_{2j})
$$
  
 
$$
\times \psi_2(\mathbf{k}_2, \mathbf{r}_{2j}) \psi_1(\mathbf{k}_1, \mathbf{r}_{1i}) d\mathbf{r}_{1i} d\mathbf{r}_{2j}
$$
  
=  $V(\mathbf{q}) | S^*(\mathbf{q}) S(\mathbf{0}) |.$  (20)

Here,  $\psi_{\alpha}(\mathbf{k},\mathbf{r})$  are the quasiparticle Bloch functions,

$$
\psi_1(\mathbf{k}, \mathbf{r}) = u_1(\mathbf{k}, \mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) \tag{21}
$$

$$
\psi_2(\mathbf{k}, \mathbf{r}) = \Omega^{-1} \exp(i\,\mathbf{k} \cdot \mathbf{r}) \tag{22}
$$

Here,  $u_1(k,r)$  is the cell periodic function which, in accordance with Eq. (2), is to be obtained by the (nearest neighbor) tight-binding approximation. The Bloch function  $\psi_2(\mathbf{k}, \mathbf{r})$  is consistent with Eq. (3).

In Eq. (20),  $V(q) = V_c(q) + V_{ph}(q)$ ; and

$$
S(\mathbf{q}) = \Omega^{-1} \int u_1(\mathbf{k} + \mathbf{q}, \mathbf{r}) \exp[i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}] d\mathbf{r} . \qquad (23)
$$

It is clear that the factor  $S(q)$  involves the band structure effects partially.

### D. A form of  $P_{nf}$

A rigorous derivation of a form of  $P_{nf}$  is a formidably difficult task so we approach this problem phenomenologically. The interaction  $V_{nf}$  will be effective in those regions of the crystal where an  $f$  atom is surrounded by its nearest-neighbor non-f atoms, because only in this region a light quasiparticle will experience change in vibrational amplitudes of atoms in going from an  $f$  atom to nearest non-f atoms. Such a change signals polarization  $P_{nf}$  due to  $V_{nf}$ . We can phenomenologically assume that  $P_{nf}$  is proportional to the amplitude ratio  $A_f/A_{nf}$ , where  $A_f$ and  $A_{nf}$  are vibrational amplitudes of an f atom and a non-f atom, respectively. In order to incorporate the effect of  $V_{nf}$  from those regions where the non-f atoms are not nearest neighbors of  $f$  atoms, we realize that all of the non- $f$  atoms of such regions will have nearly similar amplitudes and, therefore, a light quasiparticle will not see much variation in amplitudes while passing through such regions of non- $f$  atoms. Thus these non- $f$ atoms considered together will fail to maintain the  $A_f/A_{nf}$  variation of  $P_{nf}$ . That is to say, the dependence of  $P_{nf}$  on  $A_f/A_{nf}$  will be weaker than  $A_f/A_{nf}$ . Phenomenologically, we assume that  $P_{nf} = (A_f / A_{nf})^{1/\nu}$ , where  $\nu$  denotes the number of non-f atoms per f atom  $(\nu=13, e.g., in UBe<sub>13</sub>)$ . This form of  $P_{nf}$  suppresses the effect of  $V_{nf}$  for large v. Amplitudes are not measurable quantities, so we express  $P_{nf}$  in terms of masses of f and non-f atoms. For a given force constant,  $A_f \propto (M_f)^{-1/4}$ <br>and  $A_{nf} \propto (M_{nf})^{-1/4}$ , where  $M_{nf}$  is the mass of a non-j atom. This leads to the following form for  $P_{nf}$ .

$$
P_{nf} = (M_{nf}/M_f)^{1/4\nu} \tag{24}
$$

This form of  $P_{nf}$  is obtained by assuming that there is only one type of non- $f$  atoms in the heavy-fermion system. For systems like  $CeCu<sub>2</sub>Si<sub>2</sub>$  which have more than one type of non-f atoms, we shall treat  $M_{nf}$  as an average mass of different types of non-f atoms. This is because in the absence of many guidance for combining different masses, an average combination will be more reasonable than other arbitrary treatments.

Let us now analyze the sensitivity of the above phenomenological approach to  $P_{nf}$  against variation of the parameters  $M_{nf}/M_f$  and v. The minimum value of  $M_{nf}/M_f$  will correspond to that heavy-fermion system in which the  $f$  atom is the heaviest possible, and the non- $f$ atom is the lightest possible. Let the heaviest possible  $f$ atom be denoted by  $\lambda$  ( $\lambda$  corresponds to the actinides). The lightest possible non- $f$  atom, which exists in metallic form, will be that of lithium, Li. Whether  $\lambda Li_{v}$  exists as a heavy-fermion system for some  $\nu$  or not, the minimum value of  $M_{nf}/M_f$  cannot be less than that for  $\lambda Li_v$ . The value of  $\mathbf{M}_{nf}/\mathbf{M}_f$  for  $\lambda \mathrm{Li}_v$  is about  $\frac{1}{40}$ . Thus,  $P_{nf}$  will vary from  $0.4^{1/\nu}$  to 1. For real heavy-fermion systems,  $1 < v \sim 10$ , so that  $P_{nf}$  will vary from about 0.64 to 1. This variation is neither too strong nor too weak; rather, it is a mild variation. This means that the above phenomenological approach does not depend too strongly on  $P_{nf}$ through the variation of  $M_{nf}/M_f$  and v. In the absence of a realistic approach to  $P_{nf}$ , a simple approach like this will be reasonable.

## E. Features of  $J^{(11)}(q)$

The way we have expressed  $J^{(11)}(q)$  makes it clear that in this interaction the quasiparticle-phonon interaction appears at two places—one in  $V_{\text{ph}}(\mathbf{q})$  and the other in  $P_{nf}$ . Through  $V_{ph}(q)$  the quasiparticle-phonon interaction appears in the fourth order, while through  $P_{nf}$  the quasiparticle-phonon interaction appears directly in  $J^{(11)}(q)$ . This conclusion is based on the nature of simplifications used to obtain  $J^{(11)}(q)$ . In fact, within the simplifications used here, calculations show that the contribution of  $V_{\text{ph}}(\mathbf{q})$  to  $J^{(11)}(\mathbf{q})$  is at most 10% of the contribution of  $V_C(q)$ . However, the overall contribution of the quasiparticle-phonon interaction to  $J^{(11)}(q)$  will be more than this, because  $P_{nf}$  also involves the effect of the quasiparticle-phonon interaction. In most of the heavyfermion systems  $P_{nf}$  lies between 0.8 and 1. This means that the contribution of quasiparticle-phonon interaction to  $J^{(11)}(q)$  may be much higher than 10%, and the quasiparticle-phonon interaction cannot dominate over the electronic interactions in  $J^{(11)}(q)$ . This seems to be contradictory to the strong quasiparticle-phonon interaction obtained in some of the existing studies by employ-'tion obtained in some of the existing studies by employ<br>ing Kondo volume collapse<sup>2,11</sup> or other effects<sup>2,12</sup> based on electronic interactions. In fact, the point is that in other methods, first possible changes in the system due to electronic interactions are considered-the quasiparticle-phonon interaction is then calculated on the basis of such changes. On the other hand, in our method electronic and quasiparticle-phonon interactions are considered simultaneously. The main advantage of our method is that we can learn about the relative contributions of electronic and quasiparticle-phonon interactions in different heavy-fermion systems. For instance, for UPt<sub>3</sub>,  $P_{nf} \approx 1$ , and the contribution of  $V_{ph}(q)$  against  $V<sub>C</sub>(q)$  is at most 10% only. So, to a good approximation, we can treat  $UPt<sub>3</sub>$  only in terms of electronic interactions. In this way a number of models<sup>2,6</sup> based on electronic interactions are justified for  $UPt_3$  and other similar systems.

# IV. SUPERCONDUCTIVITY

According to the above treatment of interactions, heavy quasiparticles are described effectively by the effective Hamiltonian

$$
H_{\text{eff}} = H_{A1} + H_U + H_{11} \tag{25}
$$

Here,  $A_{A1}$  is that part of  $H_A$ , Eq. (1), which correspond to only heavy quasiparticles. According to Eq. (25), the heavy quasiparticles interact via the Coulomb interaction U, and via the indirect interaction  $J^{(11)}(q)$ . U is about 5,—6 eV for Ce-based systems, and about 2 eV for U-based systems.<sup>4</sup> On the other hand, the magnitude of  $J^{(11)}(\mathbf{k}_F)$ , on the basis of Sec. III, is of order 20 meV or less. This means that  $U$  is at least two orders higher in magnitude than  $J^{(11)}(q)$ . Since U is independent of q, it will have only an  $l = 0$  partial wave component, where l is an angular momentum quantum number. The  $l = 0$  partial wave component of  $\hat{J}^{(11)}(q)$  will be at most of the order of  $J^{(11)}(q)$ , and therefore, it will have much less magnitude than  $U$ . Consequently, the net contribution of  $U$  and  $J^{(11)}(q)$  to the  $l=0$  partial wave will be positive for all the heavy-fermion systems. This means that the interaction of two heavy quasiparticles in the  $l=0$  channel will be repulsive so that there cannot be s-wave (isotropicsinglet) superconductivity in heavy-fermion systems. Such a viewpoint has already been expressed in literature by many workers<sup>2,4,6,24</sup> and occurrence of supercondutivity in  $l \neq 0$  channels has been proposed.

For  $l = 0$  the contribution of  $J_K$ , Eq. (5), to a partial wave of  $J^{(11)}(q)$  becomes quite smaller than that of  $J^{(12)}(q)$ , because  $J_K$  is considered to be independent of  $q^2$ . In fact,  $J_K$  is important only for s-wave superconductivity.<sup>8</sup> So, we neglect  $J_K$  in the following development.

In order to see in which  $l > 0$  channel  $J^{(11)}(q)$  is attractive we consider its partial wave components. Let  $J_i$ denote the *l*th partial wave component of  $J^{(11)}(k_1 - k_2)$ for  $k_1 = k_2 = k_F$ .  $J_i$  is given by<sup>7</sup>

$$
J_l = 8 \int_0^1 x P_l (1 - 2x^2) J^{(11)}(2k_F x) dx , \qquad (26)
$$

where  $P_i$  is Legendre polynomial of order *l*.

Analyzing Eqs. (7), (19), (20), and (23) it can be shown that  $J^{(11)}(q)$  decreases with  $q^2$  monotonically.<sup>25</sup> This means that  $J_i$  will be negative at least for lower values of *l*. Due to increasing number of zeros of  $P_i$ , the magnitude of  $J_i$  will decrease with increasing *l*. This means that  $J_i$  will lead to the strongest attraction for  $l=1$ which corresponds to triplet pairing. Arguments in favor of  $p$  wave superconductivity already exist in literature.<sup>2,6,26</sup> The complete p-wave interaction between two heavy quasiparticles can be written as

$$
J^{(11)}(\mathbf{k}',\mathbf{k}) \approx 2J_1 F_1(\mathbf{k}')F_1(\mathbf{k}) \tag{27}
$$

where

$$
F_1(\mathbf{k}) = 2^{-1/2} A(\mathbf{k}) (|\sin k_x a + i \sin k_y a + i \sin k_z a|^2 + |\sin k_x a + i \sin k_y a - i \sin k_z a|^2)
$$
 (28)

Here,

$$
i = (-1)^{1/2},
$$
  

$$
A(\mathbf{k}) = \Theta(k_x) \Theta(k_y) \Theta(k_z) - \Theta(-k_x) \Theta(-k_y) \Theta(-k_z)
$$

with  $\Theta$  as unit step function, and "a" is lattice constant. In terms of  $J_1$  and  $F_1(k)$  the superconducting order parameter  $\Delta$  can be written as

$$
\Delta = -2J_1 \sum_{\mathbf{k}} F_1(\mathbf{k}) \langle \gamma_{1s}(-\mathbf{k}) \gamma_{1s}(\mathbf{k}) \rangle . \tag{29}
$$

Here,  $\langle \cdots \rangle$  denotes the average value in the state of the system at a given temperature T.

In order to obtain an expression for superconducting transition temperature, we diagonalize  $H_{\text{eff}}$  by introducing the antiferromagnetic order parameter

$$
M = -U \sum_{\mathbf{k}} \langle \gamma_{11}^{\dagger}(\mathbf{k} + \mathbf{Q}) \gamma_{11}(\mathbf{k}) \rangle , \qquad (30)
$$

where  $Q = G/2$  with G as reciprocal lattice vector. By diagonalizing  $H_{\text{eff}}$  we obtain

$$
1 = k_B T U \sum_{\mathbf{k}, w_n} \frac{\left[ -E_1(\mathbf{k} + \mathbf{Q}) + iw_n \right] \left[ E_1(\mathbf{k}) - iw_n \right] - \Delta^2 |F_1(\mathbf{k})|^2 + M^2}{D(\mathbf{k}, \mathbf{Q}, iw_n)}
$$
(31)

and

$$
1 = 2k_B T J_1 \sum_{\mathbf{k}, w_n} \frac{[-E_1(\mathbf{k} + \mathbf{Q}) + iw_n][E_1(\mathbf{k}) - iw_n] + \Delta^2 |F_1(\mathbf{k})| - M^2}{D(\mathbf{k}, \mathbf{Q}, iw_n)},
$$
\n(32)

with

$$
D(\mathbf{k}, \mathbf{Q}, i w_n) = [-E_1(\mathbf{k} + \mathbf{Q}) + i w_n][E_1(\mathbf{k}) - i w_n][E_1^2(\mathbf{k}) + w_n^2 + M^2 + \Delta^2 |F_1(\mathbf{k})^2|]
$$
  
+ 
$$
[E_1^2(\mathbf{k}) + w_n^2][M^2 + \Delta^2 |F_1(\mathbf{k})|^2] + [\Delta^2 |F_1(\mathbf{k})|^2 - M^2]^2.
$$
 (33)

Here,  $w_n = (2n + 1)\pi k_B T$  (with  $n = 0, \pm 1, \pm 2, \ldots$  and  $k_B$ as Boltzmann's constant) is Matsubara energy. The sum over k extends over the first Brillouin zone. The sum over the Matsubara energy  $w_n$  is restricted up to the characteristic energy  $E^{(11)}$  which was defined in the preceding section.

Equations  $(31)$ – $(33)$  allow us to learn about the superconducting order in heavy-fermion systems. The main feature of these expressions is that they characterize the superconducting order (which will appear only when  $J_1$  is significant) in a manner in which it (superconducting order) competes with the antiferromagnetic order. In fact, due to much higher temperature resistivity and magnetic susceptibility, heavy-fermion systems are expected to order magnetically at low temperatures.<sup>13</sup> If the Fermi surface nests, i.e., if  $E_1(k+Q) = -E_1(k)$  for all k, the antiferromagnetic order parameter can be quite large<sup>24</sup> so that superconductivity can be suppressed strongly. However, if the nesting of the Fermi surface is weak, the antiferromagnetic order parameter can become small enough to allow the appearance of superconductivity.

The foregoing way for treating the interaction  $U$  is based on an idea suggested earlier by Machida and Kato.<sup>24</sup> The importance of the idea of Machida and Kato lies in the fact that, as we have seen above, it can explain coexistence of antiferromagnetism and superconductivity in heavy-fermion systems (e.g., in  $URu_2Si_2$ ) Our main achievement over the work of Machida and Kato is that we have obtained an explicit form of the interaction  $J^{(11)}(q)$ , while Machida and Kato have treated teraction  $J^{(11)}(q)$ , while Machida and Kato have treated  $J^{(11)}(q)$  as a parameter. Other existing theories<sup>2,4-11</sup> of heavy-fermion superconductivity treat the interaction U in different manners without clarifying the possibility of coexistence of antiferromagnetic order and superconductivity, observed in some of the heavy-fermion systems. This means that the present theory of superconductivity is not only relativistic in terms of the interaction  $J^{(11)}(q)$ over other theories, but it also treats  $U$  in a reasonable manner.

# V. CALCULATION OF SUPERCONDUCTING TRANSITION TEMPERATURE

The mechanism of superconductivity described above depends on the process of formation of heavy quasiparticles in heavy-fermion systems in that it (the mechanism) requires knowledge of the energy bandwidths  $W_1^*$  and  $W_2^* - W_2^*$  is needed in the characteristic energy  $E^{(11)}$ (see Sec. III)—and of the value of  $U$ . But a microscopic theory of formation of heavy quasiparticles is lacking at present.<sup>2</sup> In order to avoid this problem we assume, for calculating values of the superconducting transition temperature  $T_c$  for various systems, that there is no magnetic order in the system so that in Eqs. (31)—(33) the antiferromagnetic order parameter  $M=0$ , and that the cutoff value of the Matsubara energy  $w_n$  is given by the Debye energy, rather than by  $E^{(11)}$  which needs knowledge of  $W_2^*$ . The effect of the  $M=0$  condition will be that in those systems where antiferromagnetic and superconducting orders coexist (e.g., in  $URu_2Si_2$ ), the calculate value of  $T_c$  will be higher than the actual value. Use of Debye energy as the cutoff value of  $w_n$  in Eqs. (31) and (32) is planned for the following reasons. First, Debye (32) is planned for the following reasons. First, Debye energy is expected to be of the order of  $E^{(11)}$  ( $\sim$ 200 K). Secondly, phonons contribute to  $E^{(11)}$  in an important manner. Finally, values of Debye temperature  $\Theta_D$  are known for some of the heavy-fermion systems. In fact, values of  $\Theta_D$  are known for UBe<sub>3</sub>, UPt<sub>3</sub> and UCd<sub>11</sub> which, according to Ref. 27 and to the references cited in the Table I of Ref. l, are 620, 200, and 152 K, respectively. For other systems for which calculations are made,  $CeCu<sub>2</sub>Si<sub>2</sub>$ ,  $CeRu<sub>2</sub>Si<sub>2</sub>$ ,  $CeAl<sub>3</sub>$ ,  $CeCu<sub>6</sub>$ ,  $CeB<sub>6</sub>$ ,  $URu<sub>2</sub>Si<sub>2</sub>$ , UAuPt<sub>4</sub>, U<sub>2</sub>Zn<sub>17</sub>, and UCu<sub>5</sub>, we have taken  $\Theta_D = 200$  K which is expected to give order of magnitude of  $\Theta_D$  in heavy-fermion systems. In fact, specific-heat data is known for many heavy-fermion systems, but an effort to work out a value of  $\Theta_D$  from the specific-heat data using the relation  $C_v/T = \alpha + \beta T^2$  leads to the wrong value of  $\Theta_D$ .<sup>28</sup>

We have avoided use of U and  $W_2^*$  in the present calculations at the cost of some reality of the system. But we still have a problem regarding the bandwidth  $W_1^*$ . we still have a problem regarding the bandwidth  $W_1^*$ <br>Values of  $W_1^*$  are known for some systems, <sup>17, 18</sup> but not for all the systems. We have taken different values of  $W_1^*$ ,  $W_1^* = 2$ , 2.2, 2.4, and 2.6 meV for Ce-based systems and  $W_1^* = 4, 4.5, 5,$  and 5.5 meV for U-based systems.

Other quantities involved in the calculations are approximated in the following manner. A particular Fermi wave vector  $\mathbf{k}_F \equiv (1,1,0)2\pi/3a$  has been used in the calculations. The magnitude of this  $k_F$  is consistent with the experimental values,<sup>29</sup> but is lower from the magnitudes of  $k_F$  taken by Valls and Tesanovic.<sup>6</sup> We have assumed that all the systems have simple cubic structure with the same volume per unit cell as the volume per unit cell in real systems. This choice of crystal structure makes the calculations simpler in that we can use special direction technique<sup>30</sup> for performing the integration over k in Eq. (32) by taking special directions already calculat-

TABLE I. Values of  $T_c$  for Ce-based heavy-fermion systems at various values of the bandwidth  $W_1^*$ .

	$T_c$ (K)				
System	$W_1^* = 2$ meV	$W_1^* = 2.2$ meV	$W_1^* = 2.4$ meV	$W_1^* = 2.6$ meV	
CeCu <sub>2</sub> Si <sub>2</sub>	3.02	2.42	1.39	0.00	
CeRu <sub>2</sub> Si <sub>2</sub>	3.21	2.66	1.88	0.00	
CeAl <sub>3</sub>	0.00	0.00	0.00	0.00	
CeCu <sub>6</sub>	2.61	1.90	0.00	0.00	
CeB <sub>6</sub>	3.25	2.71	1.99	1.20	

	$T_c$ (K)				
System	$W_1^* = 4$ meV	$W_1^* = 4.5$ meV	$W_1^* = 5$ meV	$W_1^* = 5.5$ meV	
$URu_2Si_2$	7.69	6.60	5.03	1.45	
$\mathbf{U}$ Be <sub>13</sub>	5.30	3.29	0.00	0.00	
UPt <sub>3</sub>	8.90	7.79	6.60	4.83	
UAuPt <sub>4</sub>	4.31	0.00	0.00	0.00	
$UCd_{11}$	0.00	0.00	0.00	0.00	
$U_2 Zn_{17}$	0.00	0.00	0.00	0.00	
UCu	7.60	6.52	4.90	0.00	

TABLE II. Values of  $T_c$  for U-based heavy-fermion systems at various values of the bandwidth  $W_1^*$ .

ed elsewhere. Values of the lattice constant are taken from Refs. 27, 31, and 32. The screening length  $1/\lambda_c$ , Eq. (6), has been treated in the random-phase approxima- $\text{tion}^{33}$  by calculating the electron density in terms of one " $(n + 1)d$ " and two " $(n + 2)s$ " electrons.

### A. Results and discussions

In searching for a superconducting order we have considered temperature values from  $T = 0.01$  to 30 K. Thus, if we do not find the solution of Eq. (32) above  $T = 0.01$ K we have concluded that the present theory does not lead to any superconducting order. Results of our calculations for  $T_c$  of various systems are shown in Tables I—III. The results of Tables I and II show that there will be no superconducting order in  $CeAl<sub>3</sub>$ , UCd<sub>11</sub>, and  $U_2 Zn_{17}$  for reasonable values of bandwidths in these systems. In other systems which we are considering, the value of  $T_c$  depends on the bandwidth  $W_1^*$  in a very strong manner. In Table III, we finally present those values of  $W_1^*$  which provide agreement with experimentally observed  $T_c$  values. These values of bandwidths are in good agreement with the experimental and theoretical values of bandwidths. $17,18$ 

We expect that the heavy-fermion systems with Cu, Au, and Pt as non-f atoms have relatively larger bandwidths. This is because the number and state of outer orbit electrons in Cu, Au, and Pt atoms are of such nature that in heavy-fermion systems the outer electron of these atoms (Cu,Au,Pt) will move in relatively wider bands

TABLE III. Values of bandwidth  $W_1^*$  for the heavy-fermion systems of Tables I and II which provide experimental values of  $T_c$ ,  $T_c^{\text{(expt)}}$  (Ref. 1).

System	$T_c^{(expt)}$ (K)	$W_1^*$ (meV)
CeCu <sub>2</sub> Si <sub>2</sub>	0.65	2.45
CeRu <sub>2</sub> Si <sub>2</sub>	< 0.01	> 2.60
CeAl <sub>3</sub>	${}_{0.01}$	>1.96
CeCu <sub>6</sub>	< 0.01	> 2.32
CeB <sub>6</sub>	< 0.01	> 2.73
$URu_2Si_2$	1.5	5.49
$UBe_{13}$	0.9	4.82
UPt <sub>3</sub>	0.5	5.88
UAuPt <sub>4</sub>	< 0.01	> 4.40
$UCd_{11}$	< 0.01	>1.13
$U_2Zn_{17}$	< 0.01	>1.92
UCu <sub>5</sub>	< 0.01	> 5.40

thereby enhancing the value of the hybridization interaction  $V$  which, in turn, will broaden the quasiparticle bands. When it is so, then according to Tables I and II, all such systems  $(CeCu_6, UAuPt_4, UCu_5)$  will fail to have superconducting order except for the system  $UPt_3$ . UBe $_{13}$ , due to its large unit cell volume, is expected to have relatively small bandwidth so that it will exhibit superconducting order. The absence of superconducting order in  $CeRu<sub>2</sub>Si<sub>2</sub>$  may be understood on the basis that although  $CeRu<sub>2</sub>Si<sub>2</sub>$  will have narrower band than  $URu<sub>2</sub>Si<sub>2</sub>$ , the difference in bandwidths cannot be large. If the bandwidth of  $URu_2Si_2$  is 5.4 meV (which, according to Table II, explains the  $T_c$  of URu<sub>2</sub>Si<sub>2</sub>), we expect the bandwidth of  $CeRu<sub>2</sub>Si<sub>2</sub>$  not less than 3 meV. According to Table I, at this bandwidth,  $CeRu_2Si_2$  will not be a superconductor. In the system  $CeB<sub>6</sub>$  the unit cell volume is less than that in other Ce-based systems which are under consideration. This means that the quasiparticle bandwidth in  $CeB<sub>6</sub>$  can be maximum among the five Ce-based systems of Table I. In fact the unit cell volume of  $CeB<sub>6</sub>$  is about half of the unit cell volume of CeAl<sub>3</sub> so that  $W_1^*$  in  $CeB<sub>6</sub>$  can be as large as 3 meV where, according to Table I, it does not have any superconducting order.

The importance of the interaction  $V_{nf}$  of a light quasiparticle with non-f atoms, which is phenomenologically accounted for by Eq. (24), becomes clear if we look at the  $T_c$  values of CeAl<sub>3</sub>, UPt<sub>3</sub>, and UBe<sub>3</sub>. CeAl<sub>3</sub> and UPt<sub>3</sub> have the same number of non-f atoms per f atom ( $v=3$ in both the systems), but an Al atom is much lighter than a Pt atom so that in CeAl<sub>3</sub> the factor  $P_{nf}$ , Eq. (24), will be much less than 1 ( $P_{nf}$ =0.8 for CeAl<sub>3</sub>), while in UPt<sub>3</sub> it will be almost 1. Consequently, the interaction  $J^{(11)}(q)$ will be significantly reduced in  $CeAl<sub>3</sub>$  and, therefore,  $CeAl<sub>3</sub>$  will fail to have a superconducting order at low temperatures. The mass of a Be atom is smaller than the mass of an Al atom, but due to the fact that the value of v is much higher in UBe<sub>13</sub> than in CeA1<sub>3</sub>, the value of  $P_{nf}$ for UBe<sub>13</sub> ( $P_{nf}$ =0.94) remains near 1 so that for a reasonable value of the bandwidths  $W_1^*$ , UBe<sub>13</sub> will be a superconducting material at low temperatures.

On the basis of the above discussion we can say that the interaction mechanism proposed here gives a reasonable explanation of the existence or absence of superconductivity in various heavy-fermion systems. Such efforts have been made earlier, also.<sup>2,4</sup> For instance, Ohkawa,<sup>5</sup> and Ohkawa and Fukuyama,<sup>5</sup> have explained the absence of superconducting order in a number of heavy-fermion systems, including CeA1 $_3$ , CeCu<sub>6</sub>, CeSn<sub>3</sub>, and CePd<sub>3</sub>, on

the basis of a deformation potential model based on the lattice structure.

#### B. Validity of calculations

Let us now consider the boundaries to the validity of the foregoing  $T_c$  calculations. As has been clarified in the preceding sections and at the beginning of Sec. V, a number of simplifications have been made in obtaining calculational expressions of  $T_c$ . Most of the simplifications are independent of each other, and so the validity criterion of the  $T_c$  calculations will involve a number of conditions which are as follows:

(i) The characteristic energy corresponding to the interaction  $\tilde{J}^{(12)}(q)$ ,  $\tilde{E}^{(12)}$ , must be much smaller in comparison to the characteristic energy  $E^{(11)}$  which corresponds to  $J^{(11)}(\mathbf{q})$ .

(ii) Below the superconducting transition temperature  $T_c$ , the system should not have any magnetic order.

(iii) Difference of the Debye energy of the solid and the characteristic energy  $E^{(11)}$  must be negligibly small.

(iv) Crystal structure effects should not be important because we have assumed only a simple cubic structure for all the systems.

(v) Spin-orbit interaction, anharmonic interaction, and retardation effects must be unimportant.

(vi) The effect of the potential field of non- $f$  atoms must be independent of the effect of the interaction  $\tilde{J}^{(12)}(q)$ , and must be neither too weak nor too strong.

(vii) Finally, the screening effect must be dominantly given by the static screening function within the random-phase approximation.

In real heavy-fermion systems some of the foregoing conditions are not satisfied, while others need justifications. In fact, conditions (iv) and (v) are not satisfied in any of the heavy-fermion systems, whereas condition (ii) is not satisfied in  $URu_2Si_2$  and  $UPt_3$ . This means that one can only regard the calculated values of  $T_c$  as very approximate ones.

#### VI. CONCLUDING REMARKS

The following conclusions can be drawn on the basis of the present study of heavy-fermion systems:

(i) A treatment of Coulomb interaction and phononmediated interaction between heavy and light quasiparticles leads to an effective interaction between heavy quasiparticles which appear to be relevant to real heavyfermion systems.

(ii) The approximation used to obtain the new effective interaction between heavy quasiparticles leave a number of unsolved problems. These problems are related mainly with the higher order terms in  $\tilde{J}^{(12)}(q)$ , with spin-orbit interaction; with crystal structure; with anharmonic interaction; with retardation effects; and with realistic details of  $V_{nf}$ .

(iii) The present approach, which ultimately is related to physical parameters of the system, is able to differentiate various heavy-fermion systems and their behavior, particularly the superconducting behavior which has been considered in this paper.

(iv) The existing controversy over whether the superconducting order is due to electronic interactions or due to phononic interaction is discussed by using the new effective interaction. This new interaction clarifies the roles of both the electronic and the phononic interactions.

(v) In the present method, calculation of  $T_c$  values needs values of the quasiparticle bandwidths  $W_1^*$ . If for some system  $W_1^*$  is not known, but  $T_c$  is known, then we can estimate  $W_1^*$  for such a system in a manner shown in Table III.

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