

## Role of Coulomb interaction in heavy-fermion systems: Calculation of effective mass

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**Abstract.** We propose a method which explicitly takes into account the strength of on-site Coulomb interactions to calculate the effective mass of carrier fermions in the intermetallics of *f* and non-*f* atoms. Calculations of a number of heavy-fermion systems show a satisfactory trend of variation of effective carrier fermion mass.

**Keywords.** On-site Coulomb interactions; heavy-fermion systems; effective mass.

### 1. Introduction

The states of the electrons in a solid are described by two limiting pictures. The usual band scheme, which is well applicable to most normal metals and semiconductors, starts with the picture of electrons moving in the periodic field of the lattice. The corresponding states (Bloch waves) are delocalized; the interaction between the electrons is usually included in the Hartree–Fock approximation. In this approximation the electrons are treated as being independent of each other and the idea of a self-consistent field is introduced. The latter is the interaction field an electron experiences when we take a spatial average over the positions of all the other electrons. On the other hand, in the case of many systems like insulating oxides of transition metals, it is more appropriate to describe the electrons in the language of localized states. This approach is applicable when there are strong inter-electronic correlations.

Nevertheless, there exist many systems (in particular, partially filled *d* and *f* states in the transition and rare earth metals and in the actinides and their compounds) that exhibit properties intermediate between the above two situations. There is general consent today that in several classes of transition metals or rare earth heavy-electron systems the *d* or *f* electrons are delocalized; it is also clear that correlations among them are not weak. Thus, a number of atomic features – like Hund's rule coupling – persist despite delocalization. Correlations are particularly strong in some of the transition metal oxides. Oxides like CoO and La<sub>2</sub>CuO<sub>4</sub> are not metallic because the

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Professor C N R Rao has had a continuing fascination and interest in metal oxides which show many interesting features arising mainly from electron correlations. We dedicate this paper to him on the occasion of his completing sixty years of age.

strong electron correlations suppress the charge fluctuations required for metallic conduction. For such systems independent electron approximation proves to be an inappropriate starting point. The competition between the localized and delocalized descriptions has been the subject of countless discussions. Whether an improved calculation should start from a wave function of the Heitler–London (strong-correlation limit) or the Hartree–Fock form (limit of independent electrons) depends on how strong electron correlations are in a given solid.

An important step to study the regime of correlated electrons was taken by Hubbard and others (Hubbard 1963, 1964) who formulated a model (the so-called one-band Hubbard model) that depends on one parameter  $U/W$ , the ratio of the short-range on-site part of the Coulomb repulsion energy  $U$  for two electrons with opposite spins, to the bandwidth  $W$  of the single-particle states. The ratio  $U/W$ , permits one to compare the effectiveness of electron interactions ( $U$ ) that favour the localized state with delocalization effects favoured by a sizable band (kinetic) energy ( $W$ ). As long as the electron correlations are weak, the residual interactions, i.e., those interactions which are not described by the self-consistent field, are small and may be treated by expansion or variational methods. The unperturbed Hamiltonian  $H_0$  is then of a single particle form. When the correlations are strong, the unperturbed Hamiltonian  $H_0$  must incorporate the dominant parts of the electron interactions, and it loses single-particle form. The main difference between a single particle Hamiltonian  $H_0$  and one which is not of a single particle form is that the Feynman diagram technique may be applied in the first but not in the second case. This is because the operators which diagonalise  $H_0$  must satisfy simple bosonic or fermionic commutation relations for Wick's theorem to hold. When  $H_0$  contains the strong electron interactions, the operators which diagonalize  $H_0$  do not satisfy the usual bosonic and fermionic commutation rules. Then the usual diagrammatic rules are not applicable. For this reason, weakly and strongly correlated electrons are treated by very different methods. We have argued elsewhere (Lamba and Joshi 1994) that it is possible to treat all possible strengths of the electron correlation by a single approach. A summary of this new variational approach applied to the Anderson lattice model is given in §2.

Here, we describe the application of this new variational approach to calculate the effective carrier fermion mass for a number of heavy-fermion systems (Grewe and Steglich 1991; Hewson 1993). Heavy-fermion systems are strongly correlated systems and are attracting interest owing to their remarkable properties. The heavy-fermion systems are metallic compounds containing  $f$ -atoms which have partially filled  $f$  orbitals (Ce, U, Np and Yb) while the other metallic constituent(s) is(are) made of non- $f$  atoms. Characteristic examples are:  $\text{CeCu}_2\text{Si}_2$ ,  $\text{CeAl}_3$ ,  $\text{CeCu}_6$ ,  $\text{CeRu}_2\text{Si}_2$ ,  $\text{CeB}_6$ ,  $\text{CePb}_3$ ,  $\text{UBe}_{13}$ ,  $\text{UPt}_3$ ,  $\text{UAuPt}_4$ ,  $\text{UPd}_2\text{Al}_3$ ,  $\text{UNi}_2\text{Al}_3$ ,  $\text{UPdSn}$ ,  $\text{UCu}_5$ ,  $\text{U}_{0.97}\text{Th}_{0.03}\text{Be}_{13}$ ,  $\text{UCd}_{11}$ ,  $\text{YbAl}_3$ ,  $\text{NpBe}_{13}$  and  $\text{YbCu}_2\text{Si}_2$ . These materials are usually described as a new class of materials; the newness is most easily characterized by a value of specific heat at low temperature, which is two to three orders of magnitude larger than values for normal metals or alloys. An increasing number of people have applied their minds to some aspect or the other of this vast and growing field. Of course, in as much as the basic problem is one of correlated electrons, it is not a new concern to condensed matter physicists.

Many problems in theoretical physics are investigated by considering mathematical models which are crude simplifications of the real situations. Such an approach can be very illuminating if the model incorporates the most important physical mechanisms

of the real problem. An excellent example of such a situation is the periodic Anderson model to study heavy-fermion systems. This model consists of a conduction band, correlated  $f$ -electron states localized at lattice sites and a hybridization ( $V$ ) between  $f$  and conduction-band electron states. In the simplest form of the model, only the spin degeneracy is taken into account.

The plan of the paper is as follows: A summary of a new variational approach applied to the Anderson lattice model (Lamba and Joshi 1994) is given in §2. Section 3 describes our method of calculation of effective hybridization and on-site Coulomb interactions. The last section (§4) highlights the simplifications used to calculate the effective carrier fermion mass for a number of heavy-fermion systems. Results and discussions are also given in the last section.

## 2. A new variational approach

The Hamiltonian for the orbitally non-degenerate periodic Anderson lattice model can be written as

$$H = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{i,\sigma} E_f \hat{n}_{fi\sigma} + V \sum_{i,\sigma} (c_{i\sigma}^\dagger f_{i\sigma} + h.c.) + U \sum_i \hat{n}_{fi\uparrow} \hat{n}_{fi\downarrow}. \quad (1)$$

The first two terms describe the broad conduction band and the non-dispersive  $f$ -level. The third term describes the hybridization between  $f$  and conduction electrons, where  $V$  denotes the hybridization matrix element which we have taken here to be a constant. The last term refers to the Coulomb interaction  $U$  between  $f$ -electrons on the same site.

The variational method essentially consists of three steps: a suitable trial state has to be devised, the expectation value of the Hamiltonian,  $\langle H \rangle$  must be evaluated and finally  $\langle H \rangle$  must be optimised.

The choice of the starting wavefunction depends on the structure of the ground state. In the non-magnetic case the starting wavefunction was taken to be the ground state wavefunction for  $H(U=0)$ .

For  $U=0$  the Hamiltonian can be easily diagonalized by the canonical transformation

$$\begin{bmatrix} c_{k\sigma} \\ f_{k\sigma} \end{bmatrix} = \begin{bmatrix} \beta'_{k\sigma} & \alpha'_{k\sigma} \\ \alpha'_{k\sigma} & -\beta'_{k\sigma} \end{bmatrix} \begin{bmatrix} u'_{k\sigma} \\ l'_{k\sigma} \end{bmatrix}, \quad (2)$$

to get the two hybridized bands

$$\xi_k^{u,l} = \frac{1}{2}(\varepsilon_k + E_f) \pm \frac{1}{2}[(\varepsilon_k - E_f)^2 + 4V^2]^{1/2}, \quad (3)$$

where  $\varepsilon_k$  and  $E_f$  are the nonhybridized and uncorrelated conduction band and  $f$ -level energy respectively. When the total number of electrons per site is taken as  $1 < n < 2$ , the ground state wavefunction in the absence of Coulomb interaction can be written as

$$|\psi_{U=0}\rangle = \prod_{k < k_{f\sigma}} l_{k\sigma}^\dagger |0\rangle. \quad (4)$$

For the finite  $U$  case we construct the trial ground state vector around the uncorrelated wavefunction by taking into account the decrease in doubly occupied sites due to the Coulomb term by introducing a projection operator  $P_i$ .

$$|\psi_c\rangle = \prod_i P_i |\psi_{uc}\rangle. \quad (5)$$

Here

$$|\psi_{uc}\rangle = \prod_{k < k_{f,\sigma}} (\alpha_{k\sigma} c_{k\sigma}^\dagger - \beta_{k\sigma} f_{k\sigma}^\dagger) |0\rangle. \quad (6)$$

$|\psi_{uc}\rangle$  is the same as  $|\psi_{U=0}\rangle$  but with  $\alpha'_{k\sigma}$  and  $\beta'_{k\sigma}$  replaced by  $\alpha_{k\sigma}$  and  $\beta_{k\sigma}$ . For the correlated problem,  $\alpha_{k\sigma}$  and  $\beta_{k\sigma}$  are to be determined variationally.

We choose the projection operator of the form

$$P_i = 1 + \sum_\sigma s_\sigma \hat{n}_{fi\sigma} - \left[ (1-d) + \sum_\sigma s_\sigma \right] \hat{n}_{fi\uparrow} \hat{n}_{fi\downarrow} \quad (7)$$

where parameter  $s_\sigma$  is introduced so that the average total density of electrons per site is conserved and  $d$  is a variational parameter which is the probability for double occupancy of a site.  $P_i$  projects out the doubly occupied sites to an extent which we determine variationally.

The ground state energy functional for the periodic Anderson model is

$$E_g = \frac{\langle \psi_c | H | \psi_c \rangle}{\langle \psi_c | \psi_c \rangle}, \quad (8)$$

where  $H$  and  $|\psi_c\rangle$  are given by (1) and (5). Various matrix elements appearing in  $E_g$  were evaluated by assuming single site approximation (SSA) (Bernasconi 1972; Oguchi 1987) and the translational invariance.

With the assumption  $n_{f\uparrow} = n_{f\downarrow} = n_f/2$  minimization of the ground state energy functional by imposing the constraint  $\alpha_{k\sigma}^2 + \beta_{k\sigma}^2 = 1$  through a Lagrange multiplier  $\lambda_{k\sigma}$  yields  $\alpha_k, \beta_k$  and  $\lambda_k$ .  $\alpha_k, \beta_k$  and  $\lambda_k$  obtained in this manner were substituted in (8) to obtain the ground state energy which can be written as

$$E_g = \frac{1}{N} \sum_{k < k_f} [(\epsilon_k + \tilde{E}_f) - [(\epsilon_k - \tilde{E}_f)^2 + 4\tilde{V}^2]^{1/2}] + \mu n_f + \frac{Ud^2 n_f^2 (1 - n_f)}{(2 - n_f)^2 - d^2 n_f^2}, \quad (9)$$

where  $\tilde{V} = VR$  is the effective hybridization energy and  $R$  is the renormalization factor which depends on the average occupation  $n_f$  in the correlated orbital and the weight factor for doubly occupied sites is given by

$$R = \frac{2(1 - n_f)(1 + s)[2 - n_f(1 - d)]}{4(1 - n_f) + (1 - d^2)n_f^2}; \quad (10)$$

$\tilde{E}_f = E_f - \mu$  is the renormalized  $f$ -level energy.  $\mu$  can be written as

$$\mu = 4V \frac{\partial R(n_f, d)}{\partial n_f} \frac{1}{N} \sum_{k < k_f} \frac{\tilde{V}}{[(\varepsilon_k - \tilde{E}_f)^2 + 4\tilde{V}^2]^{1/2}} - \frac{Ud^2}{\partial n_f} \left[ \frac{n_f^2(1-n_f)}{(2-n_f)^2 - d^2 n_f^2} \right]. \quad (11)$$

Our method of construction of the ground state energy functional is similar in spirit to that used by various authors (Rice and Ueda 1985, 1986; Vulovic and Abrahams 1987; Rice 1988).

The average occupation of  $f$ -electrons  $n_f$  is given by

$$n_f = \frac{1}{N} \sum_{k < k_f} \beta_k^2 = \frac{1}{N} \sum_{k < k_f} \left[ 1 + \frac{\varepsilon_k - \tilde{E}_f}{\{(\varepsilon_k - \tilde{E}_f)^2 + 4\tilde{V}^2\}^{1/2}} \right], \quad (12)$$

$\beta_k$  is obtained through energy minimization.

$n_f$ ,  $\mu$  and  $d$  are obtained by solving the self-consistent equations (11), (12) and  $\partial E_g / \partial d = 0$ . Detailed discussion of results for a wide range of parameters can be found in Lamba and Joshi (1994). In our model there is an enhancement of effective mass of electrons, which is given by

$$m^* = 1/VR^2. \quad (13)$$

As can be seen from (10)–(13) the effective mass depends on hybridization and Coulomb interaction in a crucial manner. A knowledge of these interactions is essential to calculate effective mass of the carrier fermions.

However, there is no reliable method to calculate the hybridization interaction and on-site Coulomb interaction in heavy-fermion systems. The main problem in the calculation of hybridization interaction is due to the fact that  $V$  (Rice and Ueda 1985, 1986; Varma *et al* 1986; Oguchi 1987; Vulovic and Abrahams 1987; Rice 1988; Lamba and Joshi 1994) depends on the intra-site Coulomb interaction between  $f$ -electrons. Therefore the first principle calculations do not yield good results even for simpler systems like UTe (Sheng and Cooper 1991). A method similar to that developed by Sheng and Cooper (1991) cannot be considered as a reliable method for heavy-fermion systems.

### 3. Method to calculate effective interactions

Instead of going to the complex problem of determination of absolute value of hybridization interaction and Coulomb interaction, we consider the calculation of relative hybridization interaction (Lal *et al* 1993) and Coulomb interaction. We incorporate the effect of non- $f$  elements through a dielectric function. So that the effective hybridization interaction  $V_{\text{eff}}$  and effective Coulomb interaction  $U_{\text{eff}}$  may be written as

$$V_{\text{eff}} = \int \frac{V(\mathbf{q})}{\varepsilon(\mathbf{q}, \omega)} d\mathbf{q} d\omega \bigg/ \int d\mathbf{q} d\omega, \quad (14)$$

$$U_{\text{eff}} = \int \frac{U(\mathbf{q})}{\varepsilon(\mathbf{q}, \omega)} d\mathbf{q} d\omega \bigg/ \int d\mathbf{q} d\omega. \quad (15)$$

Here  $\mathbf{q}$  and  $\omega$  are the electron momentum and energy respectively.

We assume that  $V(\mathbf{q}) = V_0$  and  $U(\mathbf{q}) = U_0$ .

The dielectric function  $\epsilon(\mathbf{q}, \omega)$  may be defined as (Mahan 1990)

$$\epsilon(\mathbf{q}, \omega) = \frac{v(\mathbf{q})}{v(\mathbf{q}) + v_{ph}(\mathbf{q}, \omega)} - v(\mathbf{q})P(\mathbf{q}, \omega). \quad (16)$$

Here  $v(\mathbf{q})$  is the Coulomb interaction,  $v_{ph}$  is the electron–electron interaction due to phonons, and  $P(\mathbf{q}, \omega)$  is the polarization due to  $v(\mathbf{q})$  and  $v_{ph}$ . Explicitly

$$v(q) = 4\pi e^2 / \Omega q^2, \quad (17)$$

$$v_{ph} = \frac{16\pi^2 e^2 \hbar^2}{3\Omega^2 q^2 M_{av}(\omega^2 - \omega_{ph}^2)}, \quad (18)$$

and

$$P(\mathbf{q}, \omega) = \frac{P^{(1)}(\mathbf{q}, \omega)}{1 - (v(\mathbf{q}) + v_{ph}(\mathbf{q}, \omega))P^{(1)}(\mathbf{q}, \omega)} \quad (19)$$

Here  $P^{(1)}(\mathbf{q}, \omega)$  is the polarization operator in the random-phase approximation (Mahan 1990)  $e$  is the charge of an electron,  $\Omega$  is the unit cell volume,  $\omega_{ph}$  is the phonon frequency and  $M_{av} = (M_f + vM_{nf})/(v + 1)$  is the average ionic mass in the unit cell. Here  $M_f$  and  $M_{nf}$  are the masses of  $f$ -atom and non- $f$  atom respectively, and  $v$  is the number of non- $f$  atoms per  $f$  atom in the system.

#### 4. Results and discussion

To calculate effective interactions we have made the following simplifications:

- (1) The conduction electron bandwidth and fermi energy do not depend on the nature of non- $f$  atoms.
- (2) We have neglected the details of the crystal structure by treating all the systems as having cubic structure.
- (3) The nature and occupancy of the partially filled orbitals of the non- $f$  atoms is completely ignored.
- (4) We have approximated  $P(q, \omega)$  in the random-phase approximation (Mahan 1990).
- (5) The value of  $\omega_{ph}$  is assumed to behave like  $A/M_{av}\Omega$  for all the systems. Here  $A$  is a constant which is obtained from the data of  $\text{UBe}_{13}$  (Renker *et al* 1985) ( $\omega_{ph} = 60$  meV), and is assumed to be the same for all the systems.
- (6) We have taken the following values of various parameters: half band-width  $b = 4$  eV,  $V_0 = 0.1$  eV,  $f$ -level energy  $E_f = -1.5$  eV, total density of electrons  $n = 1.6$ ,  $U_0 = 6$  eV for Ce systems and  $U_0 = 4$  eV for U systems.

We solve the self-consistent equations (11), (12) and  $\partial E_g / \partial d = 0$  using the values of  $V_{\text{eff}}$  and  $U_{\text{eff}}$  calculated by the above mentioned approach to obtain  $n_f$ ,  $d$  and  $\mu$  for various heavy-electron systems. We substitute the calculated  $n_f$ ,  $d$  and  $\mu$  in (11) and (13) to obtain the effective mass. Results of our calculations are plotted in figure 1 for a number of systems. The figure clearly shows that the trend of variation of  $m^*$

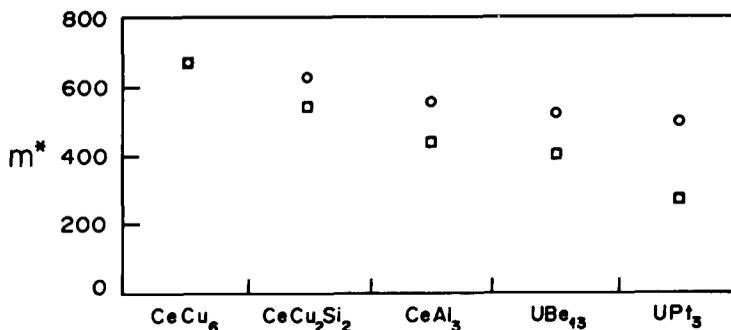


Figure 1. Calculated effective masses of the carrier fermion are compared with the experimental estimates of Fisher *et al* (1987). Squares denote the experimental estimates and circles the calculated values.

from system to system as given by present calculations does agree with that given in Fischer *et al* (1987).

In conclusion, our variational method combined with our simplified method of calculation of the effective hybridization interaction and the Coulomb interaction gives a satisfactory trend of variation of  $m^*$  in heavy-fermion systems.

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