Electronic specific heat and thermoelectric power of an Anderson lattice with finite f-band width

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(Received 4 November 1993; revised manuscript received 1 March 1994)

We study here an extension of the periodic Anderson model by considering finite f-band width. A variational method recently developed by us has been used to study the temperature dependence of the electronic specific heat C and the thermoelectric power Q for different values of the f-band width. We find that as the f-band width increases, the low-temperature peak in C becomes broader and shifts toward the high-temperature region. While the low-temperature peak in Q becomes sharper and shifts toward the low-temperature region and disappears for still larger values of the f-band width.

I. INTRODUCTION

Experimental results of electronic specific heat $C(T)$ and electrical resistivity $\rho(T)$ of many heavy fermion systems (e.g., Ce Al_3, Ce Cu_6, UBe_{13}, etc.) at low temperature show anomalous behavior (just like anomalous behavior of magnetic susceptibility at low T) in that $C(T)/T=\gamma+AT^2$ and $\rho(T)\simeq\rho(0)+BT^2$ with A and B positive (see, e.g., Refs. 1–4). The low-temperature electronic specific heat $C(T)$ of systems like Ce Al_3, Ce Cu_6, etc. show an enormous enhancement of the specific heat coefficient $\gamma(T)$ $[=C(T)/T]$, suggesting a very heavy effective mass of Fermi-liquid state. The temperature dependence of γ (T) of these compounds shows a peak $\gamma_{\max}$ at a (relatively low) temperature. The thermoelectric power $Q(T)$ also exhibits characteristic anomalies when compared to the thermoelectric power of usual metals. $Q(T)$ is very large in the case of these materials. It shows maxima at a relatively low temperature T^*. In some heavy fermion systems like U Pt_3,[5] $Q(T)$ changes sign at temperatures $T>T^*$. In the recent past, the periodic Anderson model (PAM) (Ref. 6) has been widely accepted as a model for understanding the basic electronic and magnetic properties of mixed-valence and heavy fermion materials. Since there is an overlap of $5f$ orbitals (thereby giving rise to a finite f-band width) in actinide materials,[7] we consider here an extension of the PAM by considering finite f-band width. Recently, an extension to the Anderson model in which direct f-f hopping is included has been studied by many authors.[8–10] This model has been studied by several authors using the variational method.[11–15]

We developed, recently, a variational method[16–21] to study the ground state and thermodynamic properties of PAM. We use this variational method here to study the PAM including finite f-band width. In Sec. II we give the basic formulation for electronic specific heat and thermoelectric power. In Sec. III we discuss our results.

II. BASIC FORMULATION

The orbitally nondegenerate periodic Anderson model including finite bandwidth of f electrons is described by the Hamiltonian

$$H=\sum_{k\sigma}\epsilon_k c_{k\sigma}^{+}c_{k\sigma}+\sum_{ij\sigma}T_{ij}b_{i\sigma}^{+}b_{j\sigma}-\sum_{ik\sigma}V_{ik}(c_{k\sigma}^{+}b_{i\sigma}+\text{H.c.})+\frac{U}{2}\sum_{j\sigma}n_{j\sigma}^{f}n_{j-\sigma}^{f}\ , \tag{1}$$

where

$$T_{ij}=\frac{1}{N}\sum_k E_k e^{ik(R_i-R_j)}\ . \tag{2}$$

Here E_k is the f-band energy and other symbols have their usual meanings.

For simplicity, we assume that the form of the f band is the same as that of the conduction band. The f band is represented by the expression

$$E_k=\epsilon_f+A\left[\epsilon_k-\frac{W}{2}\right]\ , \tag{3}$$

where A is some positive constant less than unity. Here W and AW are the bandwidths of conduction band and f band, respectively. For $A=0$, $E_k=\epsilon_f$ is the position of the f level.

In k-space, Anderson Hamiltonian may be written as

$$H=\sum_{k\sigma}\epsilon_k c_{k\sigma}^{+}c_{k\sigma}+\sum_{k\sigma}\left[\epsilon_f+A\left[\epsilon_k-\frac{W}{2}\right]\right]b_{k\sigma}^{+}b_{k\sigma}-\sum_{k\sigma}V_k(c_{k\sigma}^{+}b_{k\sigma}+\text{H.c.})+\frac{U}{2}\sum_{j\sigma}n_{j\sigma}^{f}n_{j-\sigma}^{f}\ . \tag{4}$$

Here we are considering strongly interacting (i.e., $U\to\infty$) case. In this case the probability of f^2 configuration is very small. The variational wave function which projects f^2 configuration out, may be written as (Panwar and Singh[16])

$$|\Psi\rangle=\prod_{k\sigma}[1+A_{k\sigma}(1-n_{-\sigma}^{f})b_{k\sigma}^{+}c_{k\sigma}]|F\rangle\ , \tag{5}$$

where $|F\rangle=\prod_{k\le k_{F,\sigma}}c_{k\sigma}^{+}|0\rangle$ is the Fermi sea of conduction electrons and $A_{k\sigma}$ the variational parameters. It can be seen that the resultant states are in the form of two quasiparticle bands; the lower $(-)$ and upper $(+)$ of quasiparticle spectra are given by

$$E_{k\sigma}^{\pm}=\frac{1}{2}\left[\left[(1+AP_f)\epsilon_k+\epsilon_f P_f-\frac{AWP_f}{2}\right]\pm\{[(1-AP_f)\epsilon_k-\epsilon_f P_f+AWP_f/2]^2+4V_k^2P_f^2\}^{1/2}\right] . \tag{6}$$

The A_k's are given by

$$A_{k\sigma}^{\pm}=\frac{1}{2V_kP_f^2}\left[\left[\epsilon_k(1-AP_f)-\epsilon_f P_f+\frac{AWP_f}{2}\right]\pm\{[\epsilon_k(1-AP_f)-\epsilon_f P_f+AWP_f/2]^2+4V_k^2P_f^2\}^{1/2}\right] \tag{7}$$

where $P_f=(1-n_{-\sigma}^f)$.

At finite temperature, the number of conduction electrons and f electrons is given by (taking total number of electrons such that Fermi level lies in the lower band)

$$n_{k\sigma}^c=\left[\frac{f_{k\sigma}^-}{1+(A_{k\sigma}^-)^2P_f^2}+\frac{f_{k\sigma}^+}{1+(A_{k\sigma}^+)^2P_f^2}\right] , \tag{8}$$

$$n_{k\sigma}^f=\left[\frac{(A_{k\sigma}^-)^2P_f^3}{1+(A_{k\sigma}^-)^2P_f^2}+\frac{(A_{k\sigma}^+)^2P_f^3}{1+(A_{k\sigma}^+)^2P_f^2}\right] . \tag{9}$$

Here, Fermi functions $f_{k\sigma}^-$ and $f_{k\sigma}^+$ are given by

$$f_{k\sigma}^{\pm}=\frac{1}{\exp[\beta(E_{k\sigma}^{\pm}-\mu)]+1} . \tag{10}$$

μ is the chemical potential and $\beta=1/k_BT$.

Let $N_\sigma^c(\epsilon_k)$ denote the density of the unperturbed conduction band, $N_\sigma^t(E_{k\sigma}^{\pm})$ the total density of lower and upper quasiparticle states, and $N_\sigma^c(E_{k\sigma}^{\pm})$ the density of (lower and upper part of) perturbed conduction states. Then

$$N_\sigma^c(E_{k\sigma}^{\pm})=\frac{N_\sigma^c(\epsilon_k)n_{k\sigma}^c}{(dE_{k\sigma}^{\pm}/d\epsilon_k)}=\frac{N_\sigma^c(\epsilon_k)}{(dE_{k\sigma}^{\pm}/d\epsilon_k)}\times\frac{f_{k\sigma}^{\pm}}{1+(A_{k\sigma}^{\pm})^2P_f^2} . \tag{11}$$

Here the factor $dE_{k\sigma}^{\pm}/d\epsilon_k$ for the lower and upper quasiparticle bands may be evaluated from Eq. (6),

$$\frac{dE_{k\sigma}^{\pm}}{d\epsilon_k}=\frac{\pm E_{k\sigma}^{\pm}\mp AP_fE_{k\sigma}^{\mp}\mp(1\pm AP_f)\left[AP_f\epsilon_k+\epsilon_fP_f-\dfrac{AWP_f}{2}\right]}{\{[\epsilon_k(1-AP_f)-\epsilon_fP_f+AWP_f/2]^2+4V_k^2P_f^2\}^{1/2}} . \tag{12}$$

A. Electronic specific heat

At finite temperature, the ground state energy is given by

$$\langle E\rangle=\sum_{k\sigma}[(E_{k\sigma}^--\mu)f_{k\sigma}^-+(E_{k\sigma}^+-\mu)f_{k\sigma}^+] . \tag{13}$$

The electronic specific heat C is obtained by differentiating energy $\langle E\rangle$ with respect to temperature T. The total specific heat gets the contribution from both the lower as well as the upper quasiparticle bands. It is given by

$$C=\frac{\partial\langle E\rangle}{\partial T}=\frac{\partial}{\partial T}\sum_{k\sigma}[(E_{k\sigma}^--\mu)f_{k\sigma}^-+(E_{k\sigma}^+-\mu)f_{k\sigma}^+] . \tag{14}$$

Equation (14) may be written as

$$C=\sum_{k\sigma}\left[f_{k\sigma}^-\frac{\partial}{\partial T}(E_{k\sigma}^--\mu)+f_{k\sigma}^+\frac{\partial}{\partial T}(E_{k\sigma}^+-\mu)+(E_{k\sigma}^--\mu)\frac{\partial f_{k\sigma}^-}{\partial T}+(E_{k\sigma}^+-\mu)\frac{\partial f_{k\sigma}^+}{\partial T}\right] . \tag{15}$$

The first two terms in the summation give the temperature dependence of quasiparticle bands, which gives a very small contribution to specific heat in the nonmagnetic case. We have neglected these two terms. The dominating terms are the third and fourth terms which give temperature dependence of Fermi function. Hence, C takes the final form.

$$C=\sum_{k\sigma}(E_{k\sigma}^--\mu)\frac{\partial f_{k\sigma}^-}{\partial T}+\sum_{k\sigma}(E_{k\sigma}^+-\mu)\frac{\partial f_{k\sigma}^+}{\partial T} . \tag{16}$$

B. Thermoelectric power

We are not interested here in the absolute value of thermoelectric power but only in the variation of thermoelectric power with temperature. The thermoelectric power $Q(T)$ may be written in the following way for both the lower and upper quasiparticle bands:

$$Q(T)=Q_0\left[\frac{\int dE_{k\sigma}^-\left[-\dfrac{\partial f_{k\sigma}^-}{\partial E_{k\sigma}^-}\right](E_{k\sigma}^--\mu)\tilde{\sigma}(E_{k\sigma}^-)}{\int dE_{k\sigma}^-(-\partial f_{k\sigma}^-/\partial E_{k\sigma}^-)\tilde{\sigma}(E_{k\sigma}^-)}+\frac{\int dE_{k\sigma}^+\left[-\dfrac{\partial f_{k\sigma}^+}{\partial E_{k\sigma}^+}\right](E_{k\sigma}^+-\mu)\tilde{\sigma}(E_{k\sigma}^+)}{\int dE_{k\sigma}^+\left[-\dfrac{\partial f_{k\sigma}^+}{\partial E_{k\sigma}^+}\right]\tilde{\sigma}(E_{k\sigma}^+)}\right] , \tag{17}$$

where $\tilde{\sigma}(E^-_{k\sigma})$ and $\tilde{\sigma}(E^+_{k\sigma})$ (Ref. 22) can be written as

$$\tilde{\sigma}(E^{\pm}_{k\sigma})=\sigma_0[N^c(E^{\pm}_{k\sigma})]^2 \tag{18}$$

and $Q_0=(1/e)$, e is the electronic charge, T is the temperature, and σ_0 is const.

III. RESULTS AND DISCUSSIONS

In these calculations, we have considered tight-binding conduction band which is centered around zero energy with conduction bandwidth $W=2.0$ eV. The total number of electrons per site (n^c+n^f) has been taken to be 1.5. The f-band width is $AW=2A$. V is fixed on 0.25 eV. The temperature is expressed in units of unperturbed conduction bandwidth W. We have calculated the temperature dependence of electronic specific heat $C(T)$ and thermoelectric power $Q(T)$ for different values of parameter A and different effective positions of the f level ϵ_f.

Figures 1(a) and 2(a) show the variation of specific heat C and specific heat coefficient C/T, respectively, with temperature for different values of parameter A. ϵ_f is fixed on -0.4. Curve I shows the variation for $A=0.0$, curve II for $A=0.05$, and curve III for $A=0.15$. In Figs. 1(b) and 2(b) we show the specific heat C and C/T, respectively, for different effective positions of f level. A is fixed on 0.05. Curve I shows the variation for $\epsilon_f=-0.4$

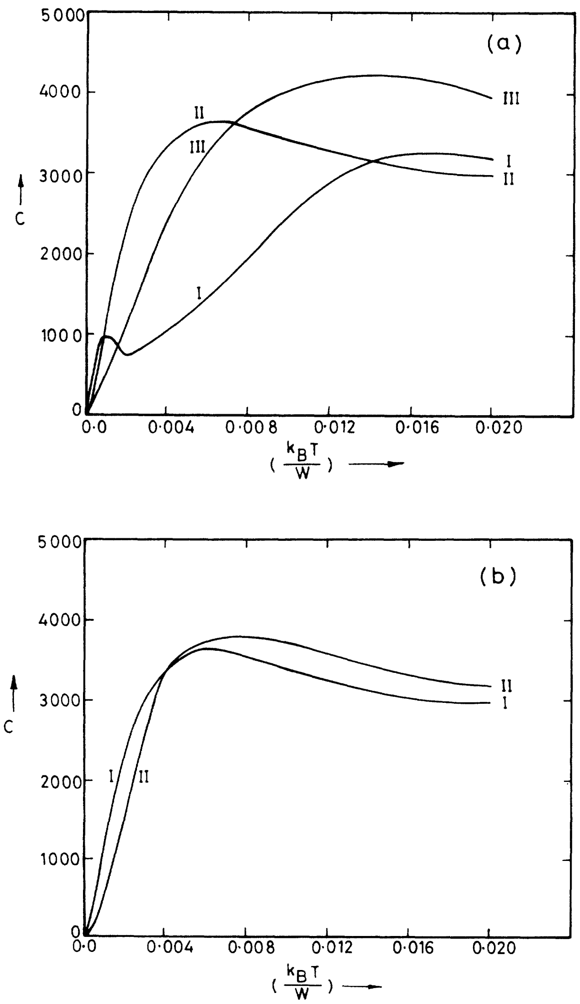

FIG. 1. Variation of specific heat C with temperature with tight-binding conduction band. $V=0.25$. (a) For different values of A. Curve I is for $A=0.0$, curve II for $A=0.05$, and curve III for $A=0.15$. ϵ_f is fixed on -0.4. (b) For different effective positions of f level. Curve I is for $\epsilon_f=-0.4$ and curve II for $\epsilon_f=0.0$. A is fixed on 0.05.

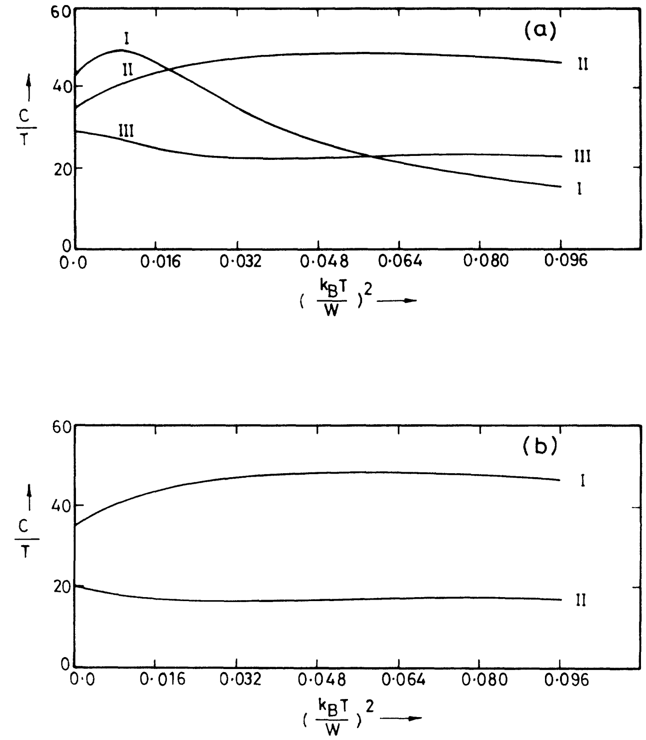

FIG. 2. Specific heat coefficient C/T as a function of temperature with tight-binding conduction band. $V=0.25$. (a) For different values of A. Curve I is for $A=0.0$, curve II for $A=0.05$, and curve III for $A=0.15$. ϵ_f is fixed on -0.4. (b) For different effective positions of f level. Curve I is for $\epsilon_f=-0.4$ and curve II for $\epsilon_f=0.0$. A is fixed on 0.05.

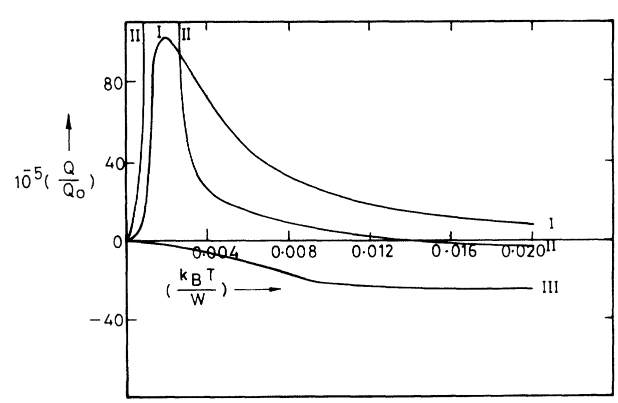

FIG. 3. Variation of thermoelectric power Q with temperature with tight-binding conduction band. $V=0.25$. $\epsilon_f=-0.4$ for different values of A. Curve I is for $A=0.0$, curve II for $A=0.05$, and curve III for $A=0.15$. The peak value of $(Q/Q_0)\times 10^{-5}$ for curve II at $(k_BT/W)=0.0012$ is 2548.

and curve II for $\epsilon_f = 0.0$. Here $C(T)$ increases linearly at low temperature and has a maximum near $T_{\max} = 12.5$ at $A = 0.0$. As A increases, the maximum is less pronounced and much broader and shifts towards higher temperature region.

Also as A increases, the maxima in C/T at low temperature becomes wider and is less pronounced and disappears in some cases. We have a sharper peak in C or C/T at low temperature as f level goes down for a constant value of A. This behavior of specific-heat curves has been the main characteristic of many mixed-valence and heavy fermion materials such as $NpSn_3$.[23]

Corresponding results for the temperature dependence of the thermoelectric power $Q(T)$ for different values of A are shown in Fig. 3. We observe maxima in $Q(T)$ at low temperature for small values of A. For some values of A (e.g., for $A = 0.05$) $Q(T)$ changes sign towards higher temperatures. The maxima in $Q(T)$ at low temperature becomes more sharper and shifts towards the low temperature region when A is increased. However, for still higher values of A, the peak disappears altogether. The behavior of $Q(T)$ for A around 0.05, corresponds to many heavy fermion compounds such as UPt_3.[5]

From the above results of $C(T)$ and $Q(T)$, one can conclude that by increasing f-band width, we are making the "Fermi-liquid" nature of f electrons more pronounced.

ACKNOWLEDGMENTS

One of the authors (S.P.) is thankful to the Council of Scientific and Industrial Research (India) for financial support. I.S. is thankful to the Department of Science and Technology (India) for financial support.

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