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Superconducting gap anomaly in heavy fermion systems

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Abstract. The heavy fermion system (HFS) is described by the periodic Anderson model (PAM), treating the Coulomb correlation between the f-electrons in the mean-field Hartree–Fock approximation. Superconductivity is introduced by a BCS-type pairing term among the conduction electrons. Within this approximation the equation for the superconducting gap is derived, which depends on the effective position of the energy level of the f-electrons relative to the Fermi level. The latter in turn depends on the occupation probability n^{f} of the f-electrons. The gap equation is solved self-consistently with the equation for n^{f}; and their temperature dependences are studied for different positions of the bare f-electron energy level, with respect to the Fermi level. The dependence of the superconducting gap on the hybridization leads to a re-entrant behaviour with increasing strength. The induced pairing between the f-electrons and the pairing of mixed conduction and f-electrons due to hybridization are also determined. The temperature dependence of the hybridization parameter, which characterizes the number of electrons with mixed character and represents the number of heavy electrons is studied. This number is shown to be small. The quasi-particle density of states (DOS) shows the existence of a pseudo-gap due to superconductivity and the signature of a hybridization gap at the Fermi level. For the choice of the model parameters, the DOS shows that the HFS is a metal and undergoes a transition to the gap-less superconducting state.

Keywords. Heavy fermion superconductor; Narrow band system; Valence fluctuation.

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1. Introduction

The discovery of superconductivity in the so-called heavy fermion system $CeCu_2Si_2$, UBe_{13}, UPt_3 [1], UNi_2Al_3 [2] and UPd_2Al_3 [3] has stimulated new efforts in the search for mechanisms for unconventional superconductivity. The neutron scattering experiments [4–6], tunneling spectroscopy [7] and NMR data [8–10] show that the systems UM_2Al_3 (M = Pd, Ni) are unconventional superconductors with node lines and very exotic pairing mechanism. The most important issue for the heavy fermion (HF) superconductors is that the quasi-particles with heavy masses ($m^* \sim 10^2 m_e$) bearing the f-electron character, condense into Cooper pairs. When we compare the phonon-mediated attractive interaction with the strong repulsive interaction among the f-electrons, it is theoretically difficult to visualize how the former interaction overcomes the latter one [11]. To avoid a large overlap of the wave functions of the paired particles, the heavy fermion systems (HFS) would rather chose an anisotropic channel, like a p-wave spin triplet or a d-wave spin singlet state to form Cooper pairs.

In these systems the pairing induced by the electron–electron interactions can be described within the Fermi liquid approach due to the possible exchange of Kondo bosons or by other pairing mechanisms based on the electronic interactions. Many authors have argued in favour of non-phonon pairing mechanisms as well as phonon pairing mechanisms (see introduction of the paper by Rout and Das [12]). Recently, some authors proposed a microscopic model for weak coupling BCS-type Cooper pairing of the conduction electrons alone in the framework of periodic Anderson model to study the temperature dependence of the SC gap in the non-magnetic HFS [12]. In this study, Coulomb correlation of the f-electrons was accounted for in mean-field approximation. Gehring and Major [13] have proposed a modified weak coupling theory of superconductivity for a uranium-based heavy fermion system where Kondo energy takes the role of cut-off. Their results show that the superconducting transition temperature is independent of the effective cut-off energy. Recently, Rout and Das have used the same weak coupling model to study the velocity of sound [14] and the Raman spectra [15] of the HF superconductors. These calculations show a deviation from BCS behaviour in the temperature dependence of the SC gap [12] in that there is a suppression of the gap throughout the temperature range with the increase in the hybridization between f-electrons and the conduction band. Furthermore, the SC gap decreases, attains a minimum and then increases with decrease of temperature in the low temperature range when the f-level is kept fixed. Such anomalies resulting from the calculations for the SC gap at low temperatures were explained earlier qualitatively. In this report, we attempt to explain quantitatively the aforesaid low temperature anomalies in the SC gap of the heavy fermion systems on the basis of the same theoretical model [12]. Because of hybridization of the f-level with the conduction band, superconducting pairing can be induced in the f-electrons as well as mixed pairing of f- and conduction electrons can be formed. Such induced superconductivity is calculated explicitly and its temperature dependence is determined. These induced pairings may contribute to the temperature dependence of the order parameter to produce the anomalous temperature dependence of the gap. An explicit demonstration of this is attempted in this paper.

The rest of the present paper is organized as follows. The model Hamiltonian for the superconductivity in the HFS is discussed in §2. The expressions for the superconducting pairing for the conduction and f-electrons are derived in §3. The results are discussed in §4 and conclusions drawn in §5.

2. Model Hamiltonian

The non-magnetic ground state of the HFS is described by the Hamiltonian $\mathcal{H}_0$ of the periodic Anderson model [12] as given below.

$$\mathcal{H}_0 = \Sigma_{k,\sigma}\epsilon_k c^\dagger_{k,\sigma}c_{k,\sigma} + \epsilon_f \Sigma_{k,\sigma} f^\dagger_{k,\sigma} f_{k,\sigma} \\ + V\Sigma_{k,\sigma}(f^\dagger_{k,\sigma}c_{k,\sigma} + c^\dagger_{k,\sigma}f_{k,\sigma}) + U/2\Sigma_{i,\sigma} n^{\mathrm{f}}_{i,\sigma} n^{\mathrm{f}}_{i,-\sigma}. \quad (1)$$

Here the first term describes the conduction electrons (in general a mixture of s, p and d states), $c^\dagger_{k,\sigma}(c_{k,\sigma})$ being the creation(annihilation) operator of the conduction electrons with momentum k and spin σ and ϵ_k is the conduction band energy. Similarly, $f^\dagger_{k,\sigma}(f_{k,\sigma})$ is the on-site creation(annihilation) operator for the f-electron. The third term describes the hybridization of f-states with the conduction electrons on the same site. The quantity ϵ_f is the bare f-level position and V is the strength of the hybridization between f-level and the conduction band. The last term describes intra-atomic Coulomb interaction between the f-electrons. Here $n^{\mathrm{f}}_{i,\sigma} = f^\dagger_{i,\sigma}f_{i,\sigma}$ is the number operator for f-electrons. The on-site f-electron interaction terms $n^{\mathrm{f}}_{i,\sigma}n^{\mathrm{f}}_{i-\sigma}$ in the Hamiltonian $\mathcal{H}_0$ is usually very strong in these HF systems and has a strength U. However, for simplicity this term is treated in the mean-field Hartree–Fock approximation in this paper. Within this approximation $n^{\mathrm{f}}_{i,\sigma}n^{\mathrm{f}}_{i-\sigma} \simeq n^{\mathrm{f}}_{i,\sigma}\langle n^{\mathrm{f}}_{i-\sigma}\rangle + \langle n^{\mathrm{f}}_{i,\sigma}\rangle n^{\mathrm{f}}_{i-\sigma}$ and the two-electron interaction is replaced by single-electron operators which essentially renormalize the energy of the f-level. The main advantage of this approximation is that the resulting many-body problem becomes exactly solvable, at the cost of missing the consequences of strong correlation physics, like metal–insulator transition. Since we are looking at mainly the superconductivity within the BCS framework in the HF systems, the mean-field approximation is justifiable. This reduces the Hamiltonian to that of a collection of non-interacting electrons with a modified f-level with energy, $E_0 = (\epsilon_f + Un_{-\sigma})$ where $n_{-\sigma} = \langle n_{i-\sigma}\rangle$ independent of the site. A weak coupling BCS-type pairing mechanism between the conduction electrons is introduced as a model to account for the superconductivity observed in some of the HF systems. The BCS Hamiltonian is given by

$$\mathcal{H}_I = -\Delta\Sigma_k(c^\dagger_{k,\uparrow}c^\dagger_{-k,\downarrow} + c_{-k,\downarrow}c_{k,\uparrow}), \quad (2)$$

where Δ is the superconducting order parameter independent of wave vector k, corresponding to the S-wave pairing.

3. Expression for gap equation

The single particle c- and f-electron Green's functions are calculated using Zubarev's technique [16] by writing the equation of motion. The exact solution involves a set of four coupled equations for c-electron Green's functions and another set of four coupled equations for the f-electron Green's functions which are solved separately. The SC gap parameter and other correlation functions are calculated from these eight Green's functions. The gap equation for the Cooper pair binding $\Delta(T)$ is defined as

$$\Delta(T) = -\Sigma_k \tilde{V}_k [\langle c^{\dagger}_{k,\uparrow} c^{\dagger}_{-k,\downarrow} \rangle + \text{h.c.}] = -\Sigma_k [\tilde{V}_k \phi^{\mathrm{c}}_k + \tilde{V}^*_k \phi^{\mathrm{c}*}_k], \tag{3}$$

where ϕ^{c}_k is the superconducting (SC) pairing amplitude of the conduction electrons and $\tilde{V}_k$ (also taken to be a constant V_0) is the effective attractive interaction.

Although the HF systems are known to be anisotropic superconductors, it is hoped to gain some insight into the problem from this study of the simplified weak coupling and conventional pairing mechanism. The parameter Δ is calculated to give the gap equation as

$$1 = g_1 \int_{-\omega_D}^{\omega_D} \mathrm{d}\epsilon_k \frac{1}{2(\omega_1^2 - \omega_2^2)} \left[E_1(\epsilon_k, T) - E_2(\epsilon_k, T) \right], \tag{4}$$

where

$$E_1(\epsilon_k, T) = \frac{\omega_1^2 - E_0^2}{\omega_1} \tanh\left(\frac{\beta\omega_1}{2}\right),$$
$$E_2(\epsilon_k, T) = \frac{\omega_2^2 - E_0^2}{\omega_2} \tanh\left(\frac{\beta\omega_2}{2}\right). \tag{5}$$

The poles of the Green's functions give four quasi-particle energy bands $\pm\omega_i(\epsilon_k)$ (with $i = 1, 2$) which are given by

$$\omega_{1,2}(\epsilon_k) = \left[\frac{R \pm \sqrt{R^2 - 4S}}{2} \right]^{1/2}, \tag{6}$$

where

$$R = E_0^2 + E_k^2 + 2V^2, \quad S = E_0^2 E_k^2 - 2\epsilon_k E_0 V^2 + V^4, \quad E_k^2 = \epsilon_k^2 + \Delta^2$$

and

$$E_0 = \epsilon_f + U n_{-\sigma} = \epsilon_f + U n_f / 2. \tag{7}$$

The last equality in eq. (7) assumes $n_{-\sigma} = n_f/2$ since the system under consideration is non-magnetic. In eq. (4) Σ_k is replaced by an integration over energy $\int N(0) \mathrm{d}\epsilon_k$ with the integration limits going from $-\omega_D$ to $+\omega_D, \omega_D$ being some cut-off energy where $N(0)$ the density of states of the conduction electrons at the Fermi level ϵ_{F} is taken to be constant and the superconducting coupling constant $g_1 = V_0 N(0)$. It can be seen from eq. (4) that the superconducting gap depends explicitly on the effective position of the f-level E_0, hybridization strength V and electronic repulsion U, which are characteristics of the HFS. The f-level energy E_0 in turn depends on the occupation probability n^{f} of the f-level which is a temperature-dependent quantity. Therefore, it is expected that superconductivity in the HF systems will be effected by the position of the f-level relative to the Fermi level at a particular temperature. In the absence of the hybridization the conduction electrons and the f-electrons will decouple and behave as independent entities. So the superconductivity will not be influenced by the f-electrons present in the system. Even though the Cooper pairing is introduced in the conduction electrons alone, the hybridization between the conduction and f-electrons, ultimately induces pairing in the f-electrons as well. The mixed pairing Δ_1 between the f-electron and conduction electron is defined as $\Delta_1 = \Sigma_k[\langle c^\dagger_{k,\uparrow} f^\dagger_{-k,\downarrow}\rangle + \text{h.c.}] = \Sigma_k[\psi_k + \psi^*_k]$ where ψ_k is the mixed Cooper pairing amplitude between c- and f-electrons. Using the Green's function, Δ_1 is calculated as

$$\Delta_1 = N(0) \int_{-\omega_D}^{\omega_D} \mathrm{d}\epsilon_k \frac{\Delta V E_0}{2(\omega_1^2 - \omega_2^2)} \left[E_3(\epsilon_k, T) - E_4(\epsilon_k, T)\right], \tag{8}$$

where

$$E_3(\epsilon_k, T) = \frac{1}{\omega_1} \tanh\left(\frac{\beta\omega_1}{2}\right), \quad E_4(\epsilon_k, T) = \frac{1}{\omega_2} \tanh\left(\frac{\beta\omega_2}{2}\right). \tag{9}$$

Similarly, due to the presence of hybridization, the induced f-electron pairing Δ_2 which is defined as $\Delta_2 = \Sigma_k[\langle f^\dagger_{k,\uparrow} f^\dagger_{-k,\downarrow}\rangle + \text{h.c.}] = \Sigma_k[\phi^{\mathrm{f}}_k + \phi^{\mathrm{f}*}_k]$ where ϕ^{f}_k is the f-electron Cooper pairing amplitude, is given by

$$\Delta_2 = -N_f(0) \int_{-\omega_D}^{\omega_D} \mathrm{d}\epsilon_k \frac{\Delta V^2}{2(\omega_1^2 - \omega_2^2)} \left[E_3(\epsilon_k, T) - E_4(\epsilon_k, T)\right]. \tag{10}$$

The induced pairing amplitudes Δ_1 and Δ_2 depend on both the hybridization parameter V and the superconducting order parameter Δ as can be seen from eqs (8) and (10). In the absence of any one of them these quantities vanish as expected. Yet another quantity $\lambda = -\Sigma_k[\langle c^\dagger_{k,\sigma} f_{k,\sigma}\rangle + \text{h.c.}]$ which exists because of hybridization both in the normal state and the SC state is also calculated. The average value of this parameter in the normal state gives the hybridization gap and is responsible for the heavy fermion behaviour. The hybridization parameter λ is found to be

$$\lambda = N(0) \int_{-W/2}^{W/2} \mathrm{d}\epsilon_k \frac{V}{(\omega_1^2 - \omega_2^2)} \left[E_5(\epsilon_k, T) - E_6(\epsilon_k, T)\right], \tag{11}$$

where

$$E_5(\epsilon_k, T) = \frac{\omega_1^2 + \epsilon_k E_0 - V^2}{\omega_1} \tanh\left(\frac{\beta\omega_1}{2}\right),$$

$$E_6(\epsilon_k, T) = \frac{\omega_2^2 + \epsilon_k E_0 - V^2}{\omega_2} \tanh\left(\frac{\beta\omega_2}{2}\right). \tag{12}$$

The other quantities of interest are the occupation number n^{f} of the f-electrons and n^{c} of the conduction electrons which are also calculated and given by

$$n^{\mathrm{f}} = \Sigma_k \left[1 - \frac{1}{(\omega_1^2 - \omega_2^2)} \{E_7(\epsilon_k, T) - E_8(\epsilon_k, T)\} \right], \tag{13}$$

where

$$E_7(\epsilon_k, T) = \frac{\omega_1^2 E_0 - E_0 E_k^2 + \epsilon_k V^2}{\omega_1} \tanh\left(\frac{\beta\omega_1}{2}\right)$$

$$E_8(\epsilon_k, T) = \frac{\omega_2^2 E_0 - E_0 E_k^2 + \epsilon_k V^2}{\omega_2} \tanh\left(\frac{\beta\omega_2}{2}\right) \tag{14}$$

$$n^{\mathrm{c}} = \Sigma_k \left[1 - \frac{1}{(\omega_1^2 - \omega_2^2)} \{E_9(\epsilon_k, T) - E_{10}(\epsilon_k, T)\} \right], \tag{15}$$

where

$$E_9(\epsilon_k, T) = \frac{\omega_1^2 \epsilon_k - \epsilon_k E_0^2 + E_0 V^2}{\omega_1} \tanh\left(\frac{\beta\omega_1}{2}\right),$$

$$E_{10}(\epsilon_k, T) = \frac{\omega_2^2 \epsilon_k - \epsilon_k E_0^2 + E_0 V^2}{\omega_2} \tanh\left(\frac{\beta\omega_2}{2}\right). \tag{16}$$

It should be noted that the total number of electrons per atom (n^{t}) is fixed and given by $n^{\mathrm{f}} + n^{\mathrm{c}} = n^{\mathrm{t}}$. Hence, if we calculate the temperature dependence of n^{f} then that of n^{c} is automatically given by $n^{\mathrm{c}} = n^{\mathrm{t}} - n^{\mathrm{f}}$, and it need not be explicitly evaluated from eq. (15). On the other hand, in the superconducting state, $n^{\mathrm{f}}(T)$ depends on the gap parameter $\Delta(T)$ through the energy E_k; while the SC gap $\Delta(T)$ depends on $n^{\mathrm{f}}(T)$ through the effective f-electron energy E_0, hence $\Delta(T)$ and $n^{\mathrm{f}}(T)$ have to be calculated self-consistently keeping the other parameters like ϵ_f, V and g_1 fixed. In what follows we shall implement the self-consistent solution of eqs (4) and (13) numerically.

The parameters involved in the calculation can be scaled by one of the suitable energies associated with the HFS, i.e. the superconducting transition temperature $T_{\mathrm{c}} \approx 1$ K, keeping with the weak coupling theory the cut-off frequency is taken to be $\omega_D \approx 200$ cm^{-1} and the conduction band width is around $W \approx 1$ eV to understand the influence of the other correlations like Δ_1, Δ_2 and λ on the SC gap parameter. In what follows the parameters are scaled by cut-off frequency ω_D which, in turn, makes them dimensionless. Keeping in mind the fact that superconductivity appears at low temperatures, the gap parameters and the variable temperature are also measured with respect to the cut-off frequency ω_D. Similarly, since we shall be looking for effects like induced pairing in the f-electrons, which are expected to depend sensitively on how close is the f-level to the Fermi level and how strong is the hybridization, we choose to scale the hybridization strength as well with the cut-off frequency. That leaves the Coulomb interaction U, which can be scaled with respect to the bandwidth W. Since the Coulomb repulsion between the f-electrons is treated in the mean-field approximation, it is implicitly assumed that the correlations are weak.

Therefore we scale all the parameters with ω_D and shall choose reasonable values for u and v, the Coulomb repulsion and the strength of the hybridization respectively to make them physically acceptable. The dimensionless parameters are

$$d = \frac{\epsilon_f}{\omega_D}, \quad u = \frac{U}{\omega_D}, \quad v = \frac{V}{\omega_D}, \quad g_1 = N(0)V_0, \quad t = \frac{k_B T}{\omega_D}, \quad z = \frac{\Delta}{\omega_D}$$

The parameters d, u and v are so chosen that they remain within the limits of the integration which goes from $-\omega_D(\simeq -1)$ to $+\omega_D(\simeq +1)$ in the evaluation of the SC gap. Furthermore, for the f-level to effect the superconductivity it should be close to Fermi level. In what follows the choice of the values of these parameters may look like unphysically small, but it should be kept in mind that by increasing the bandwidth W and the cut-off frequency ω_D the parameters can be made as large as required. For example, one can make the Coulomb repulsion U large and push the f-level ϵ_f away from the Fermi level so that the effective f-level position E_0 remains near the Fermi level.

4. Results and discussion

The temperature dependence of the SC gap for the HFS within this theoretical model can be studied by varying different model parameters of the system, i.e. superconducting coupling strength (g_1), position of bare f-level (d), Coulomb interaction (u) and hybridization (v) as a function of the reduced temperature (t). The SC gap parameter (z) as well as the f-electron occupation number n^{f} are determined numerically following a self-consistent procedure. The gap equation for z in dimensionless form is integrated from -1 to $+1$. The temperature variation of the order parameter z and other quantities like $z_1(\Delta_1/\omega_D), z_2(\Delta_2/\omega_D)$ and λ are used to interpret the HF superconductivity choosing a standard set of values for the parameters $g_1 = 0.18435$, $u = 0.01$ and $v = 0.0035$.

In this paper an extremely simplified model is presented for the HFS and its superconductivity. The normal state of the HFS is described by the periodic Anderson model, and its superconductivity by introducing a BCS-like term in the Hamiltonian for the conduction electrons. It is further simplified by treating the strong electronic correlation between the f-electrons within the mean-field Hartree–Fock approximation. The consequence of this is to modify the effective position of the f-level; which in the dimensionless form takes the value $d_1 = d + un^{\mathrm{f}}_{-\sigma}$. Since we are dealing with a non-magnetic system $n^{\mathrm{f}}_{-\sigma} = n^{\mathrm{f}}_{\sigma} = n^{\mathrm{f}}/2$ and $d_1 = d + un^{\mathrm{f}}/2$. Thus the effective d-level acquires a temperature dependence through n^{f}. The occupation of the f-level is determined self-consistently by solving the coupled equations for $\Delta(T)$ and $n^{\mathrm{f}}(T)$ together. It is expected that the superconducting gap will be influenced by the f-level only when the latter is close to the Fermi level. In the present calculation the energy of the conduction orbital is taken to be zero ($\epsilon^{\mathrm{c}}_0 = 0$), and so all the energies are measured from the Fermi level ($\epsilon_{\mathrm{F}} = 0$). Furthermore, it is assumed that there is one conduction electron and one f-electron per atom in the system. So we have the constraint $n^{\mathrm{f}} + n^{\mathrm{c}} = 2$, which may correspond to the conduction band being half filled with the band spreading symmetrically around the Fermi level. The f-level which can be thought of as half empty can lie either just below or just above ϵ_{F} in order to effect the superconductivity and the Cooper pairing in the conduction band. If it is too deep below the Fermi level, thermal fluctuation cannot promote the f-electrons to the conduction band states which are already occupied, due to Pauli blocking. Similarly, the conduction electrons cannot gain in energy by jumping into the empty states of the f-level, because of the strong Coulomb repulsion due to double occupancy. On the other hand, if the f-level is above the Fermi level it is expected that the f-level can lower the energy of the system by moving over to occupy the empty conduction band states between $\epsilon_{\rm F}$ and $\epsilon_{\rm f}$, i.e. $\epsilon_{\rm f} > \epsilon > \epsilon_{\rm F}$. Thus the Fermi level will get pinned to the f-level. However, with increasing temperature thermal fluctuations will tend to populate the f-level by conduction electrons, thereby increasing the f-electron number. This will involve the breaking of Cooper pairs and hence the suppression of the superconducting gap. Thus, only if the f-level is either above or below, but close to the Fermi level then its presence can effect the superconducting order parameter. These are some of the intuitive expectations for the consequences of the simple model.

To verify these expectations the SC gap eq. (4) and the equation for $n^{\rm f}$ eq. (13) are solved numerically self-consistently, for different values of the f-level position d. The other parameters of the model are kept fixed as mentioned above. The values of d (all below the Fermi level) are so chosen that the effective position d_1 of the f-level can be either above or below $\epsilon_{\rm F}$. The temperature dependence of $n^{\rm f}$ and consequently that of the effective f-level d_1 are shown in figures 1 and 2 respectively for a choice of the bare f-level energy d going from -0.0006 to -0.0086. While all these values of d correspond to the bare f-level being below $\epsilon_{\rm F}$, the first two are close to the Fermi level, so that the effective f-level d_1 goes above the Fermi level. As expected for these two d-values the occupation $n^{\rm f}$ is depleted at zero temperature $t = 0$ and gradually increases with increasing temperature. For all other d values d_1 is negative, the effective f-level being deep down from $\epsilon_{\rm F}$ for the last two values of d. For the latter cases the f-level is fully occupied at zero temperature and the occupation decreases with increasing temperature. So the trends of the temperature dependence are different when the effective d-level is above or below $\epsilon_{\rm F}$. The optimum case will be for quarter filling of the f-level, which will correspond to $d = -0.0025$ and in this case the Fermi level will be pinned to the f-level at all temperatures.

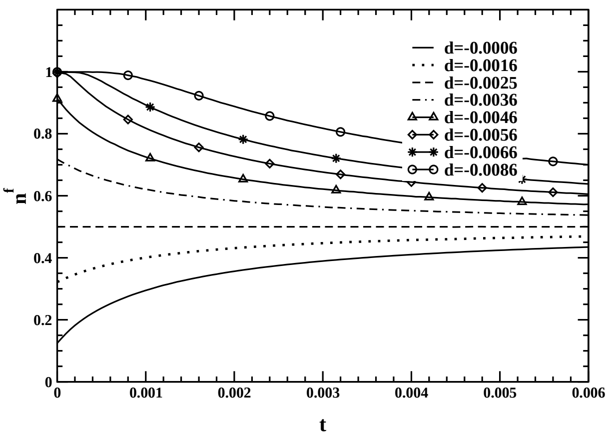

Figure 1. Plot of $n^{\rm f}$ vs. temperature t for different values of $d = -0.0006, -0.0016, -0.0025, -0.0036, -0.0046, -0.0056, -0.0066, -0.0086$ with fixed values of $u = 0.01, v = 0.0035$, $g_1 = 0.18435$.

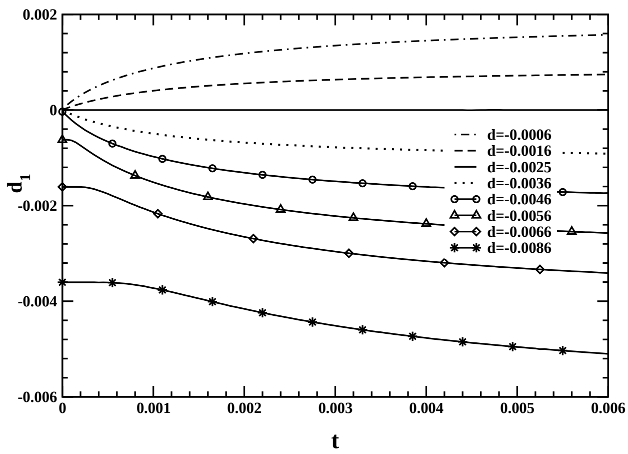

Figure 2. Plot of effective f-level position d_1 vs. temperature t for different values of $d = -0.0006, -0.0016, -0.0025, -0.0036, -0.0046, -0.0056, -0.0066$ and -0.0086 with fixed values of $u = 0.01, v = 0.0035$, $g_1 = 0.18435$.

The temperature dependence of the superconducting gap parameter z for different values of d is depicted in figure 3. When the f-level is too deep below the Fermi level as in case of $d = -0.0086$, the temperature dependence at low temperatures more or less shows the BCS-like behaviour except for the fact that its magnitude is slightly reduced when compared with the BCS result corresponding to the case of vanishing hybridization ($v = 0$) which is depicted in figure 4. In the absence of hybridization the conduction electrons are decoupled from the f-electrons, hence the latter do not effect the superconductivity in the system. With the f-level moving towards the Fermi level there is an overall suppression in superconductivity, the effect being more prominent at low temperatures as can be seen from figure 3.

In some cases the suppression even takes the form of a dip, e.g. $d = -0.0056$. An overall consequence of this is that the ratio $2\Delta(0)/k_{\mathrm{B}}T_{\mathrm{c}}$ decreases from its standard BCS value of 3.52. While it may look too far fetched to compare this result with experimental data for the system UPd_2Al_3, this ratio is 2.2 as determined from neutron scattering measurements. However, the value determined from other measurements like tunneling spectroscopy and NMR and Knight shift give values higher than that of the BCS value. It is worth noting from figure 3 that the trends in the low temperature suppression of the superconducting gap are different when the effective f-level is above the Fermi level than when it is below. For example, when d goes from -0.0006 to -0.0016, the effective f-level d_1 moves towards the Fermi level (figure 2) with increasing temperature and the suppression in the SC gap increases. But when d moves from -0.0056 to -0.0086 resulting in the effective f-level d_1 getting below the Fermi level and moves deeper into the conduction electron Fermi sea, the low temperature suppression in the gap decreases. This again indicates that, how the presence of the f-electron effects superconductivity depends very much on where the effective f-level lies; above or below the Fermi level; which in turn depends on the Coulomb interaction between the localized f-electrons. It should be pointed out that the self-consistently determined temperature dependence

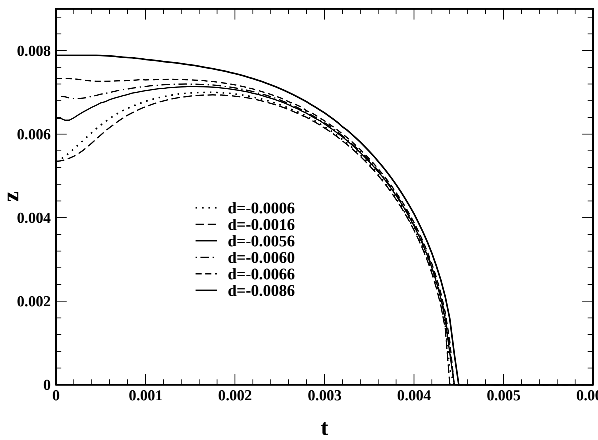

Figure 3. Plot of superconducting gap z vs. temperature t for different values of $d = -0.0006, -0.0016, -0.0056, -0.0060, -0.0066, -0.0086$ with fixed values of $u = 0.01, v = 0.0035,\ g_1 = 0.18435$.

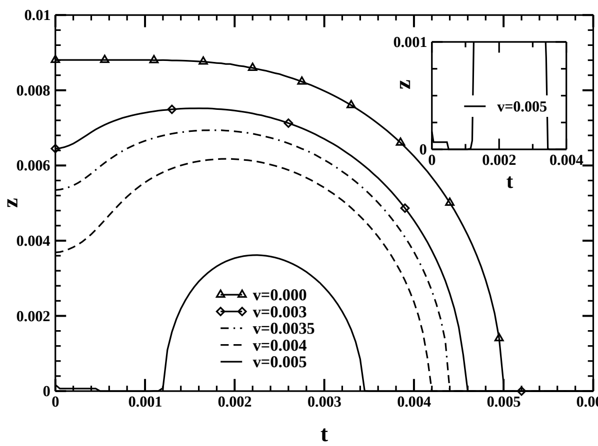

Figure 4. Plot of superconducting gap z vs. temperature t for different values of $v = 0.000, 0.003, 0.0035, 0.004, 0.005$ with fixed values of $d = -0.0016, u = 0.01,\ g_1 = 0.18435$. The inset shows the same graph for $v = 0.005$.

of the f-electron occupation (figure 1) turns out to be independent of the value of the strength of the hybridization parameter v.

The effect of the variation of the strength of the hybridization (v) on the temperature dependence of the SC gap (z) is shown in figure 4. As can be seen from the figure, this effect is much more dramatic compared to the effect of d on the temperature dependence of z. With increasing v not only the SC order parameter is suppressed through out the temperature range with large suppression at low temperatures, but also for large value of v (=0.005) the system shows re-entrant behaviour. The superconductivity is completely suppressed below a certain temperature

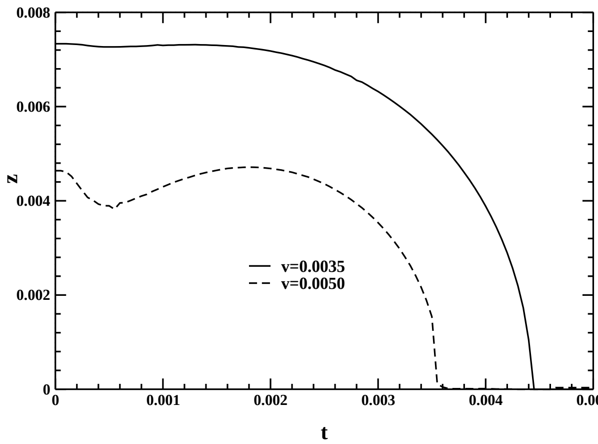

Figure 5. Plot of superconducting gap z vs. temperature t for different values of $v = 0.0035, 0.005$, with fixed values of $d = -0.0066, u = 0.01$, $g_1 = 0.18435$.

and then reappears again near zero temperature with much smaller magnitude, as shown in the inset. Further increase in the strength of the hybridization destroys superconductivity completely. Comparing the low temperature behaviour of the z vs. t curves in figures 4 and 3 one will be tempted to remark that the low temperature dip in z in figure 3 can be attributed to the effect of hybridization and is a precursor to the appearance of the re-entrant behaviour, as can be seen from figure 5, when the value of d is decreased from $d = -0.0016$ (figure 4) to $d = -0.0066$ (figure 5).

It is really puzzling as to why there is an overall suppression of the superconducting gap z over the entire temperature range $t < t_{\mathrm{c}}$; both with increasing value of the position of the bare f-level (d) and with the increasing strength of the hybridization (v)? It is well-known that when there is co-existence of two long range orders, the order parameter of the one with the higher transition temperature is suppressed in a discontinuous manner at the temperature where the second long range order appears, and this suppression continues till the temperature goes to zero. Well-known example of such behaviour is the co-existence of structural transition and superconductivity [**?**]. In this case the structural transition is arrested when superconductivity appears in the system. In contrast to this behaviour here the superconducting order parameter is continuously suppressed on lowering the temperature, in the absence of the emergence of a second long range order. There is the possibility of the appearance of gap or a pseudo-gap due to the hybridization which will result in the suppression of the density of states at the Fermi level, resulting in the suppression of the superconductivity. Furthermore, due to the hybridization there may be induced pairing of the f-electrons and the mixed pairing of the conduction and the f-electrons in addition to the Cooper pairing of the conduction electrons. All these effects could influence the observed superconductivity in the system. In what follows we explore these possibilities. We calculate the induced Cooper pairing amplitudes for mixed pairing $\psi_k = \langle c^{\dagger}_{k\uparrow} f^{\dagger}_{-k\downarrow} \rangle$, and the

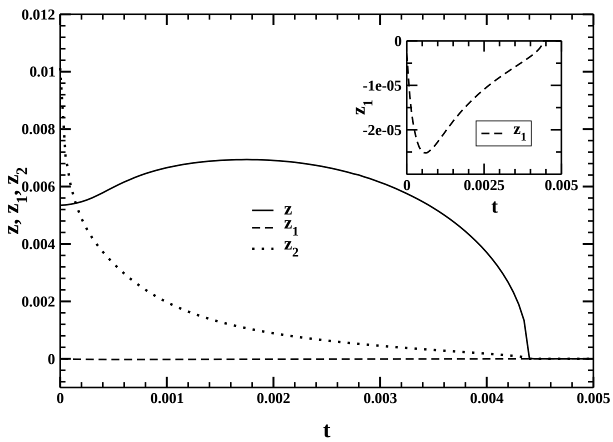

Figure 6. Plot of superconducting gap z, z_1, z_2 vs. temperature t with fixed values of $d = -0.0016, u = 0.01, v = 0.0035$, $g_1 = 0.18435$. The inset shows the plot for z_1.

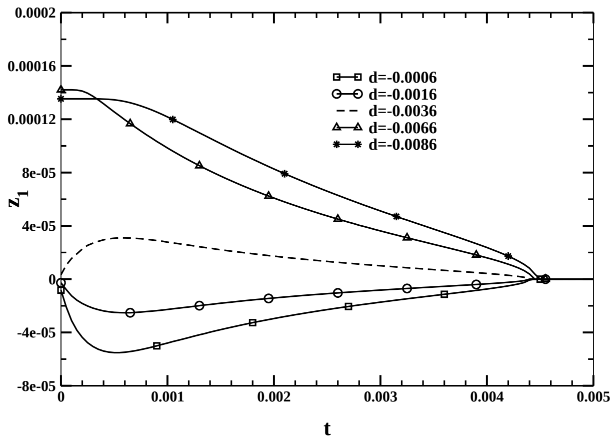

Figure 7. Plot of superconducting gap z_1 vs. temperature t for different values of $d = -0.0006, -0.0016, -0.0036, -0.0066, -0.0086$ with fixed values of $u = 0.01, v = 0.0035$, $g_1 = 0.18435$.

corresponding gap parameter Δ_1 (z_1 in dimensionless form) from eq. (8), the f-electron pairing amplitude $\phi_k^{\mathrm{f}} = \langle f_{k\uparrow}^{\dagger} f_{-k\downarrow}^{\dagger} \rangle$ and the corresponding gap parameter Δ_2 (denoted as z_2 in dimensionless form) from eq. (10), and the hybridization parameter λ, whose amplitude $n_k^{\mathrm{c-f}} = \langle c_{k\sigma}^{\dagger} f_{k\sigma} \rangle$ from eq. (11) for the standard set of values for the parameters $g_1 = 0.18435$, $u = 0.01$ and different values of the positions of the bare f-level (d) and the strength of hybridization (v), as used in the calculation of z, to facilitate the comparison.

The temperature dependence of z, z_1 and z_2 for $d = -0.0016$ and $v = 0.0035$ are shown in figure 6. As expected the magnitudes of the induced gap parameters z_1 and z_2 below t_{c} are much smaller than that of z. While z_1 remains negligibly small

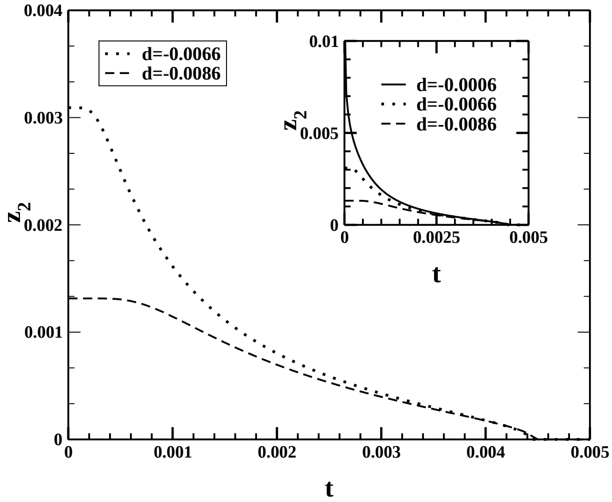

Figure 8. Plot of superconducting gap z_2 vs. temperature t for different values of $d = -0.0066, -0.0086$ with fixed values of $u = 0.01$, $v = 0.0035$, $g_1 = 0.18435$. The inset shows the same plot for $d = -0.0006, -0.0066, -0.0086$.

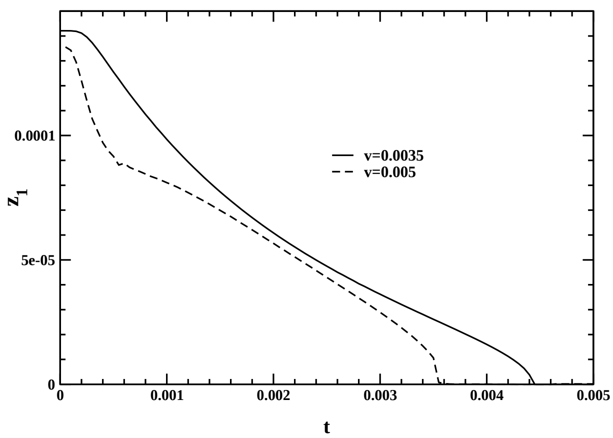

Figure 9. Plot of superconducting parameter z_1 vs. temperature t for different values of $v = 0.0035, 0.005$ with fixed values of $d = -0.0066, u = 0.01$, $g_1 = 0.18435$.

(and negative for this d value) up to $t = 0$, z_2 increases rapidly as t approaches 0 K and even exceeds the value of z. On the other hand, z_1 has a dip near 0 K, as shown in the inset of figure 6. As the bare f-level moves down from the Fermi level, z_1 becomes positive but still remains small as can be seen from figure 7.

At the same time the magnitude of z_2 near $t = 0$ decreases as d moves deeper from the Fermi level as shown in figure 8 and its inset. Under these latter conditions the f-level is fully occupied (see figure 1) at low temperatures because of which putting

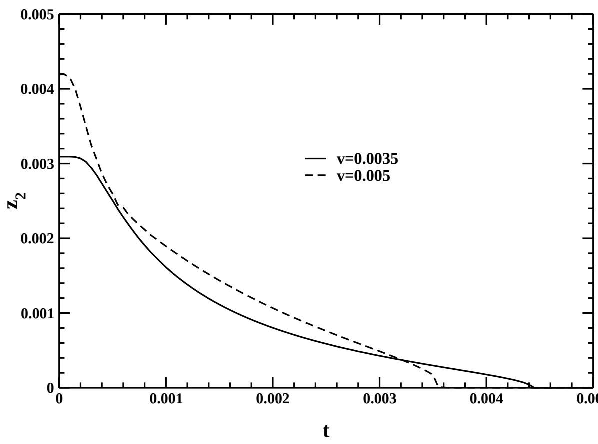

Figure 10. Plot of superconducting parameter z_2 vs. temperature t for different values of $v = 0.0035, 0.005$ with fixed values of $d = -0.0066, u = 0.01$, $g_1 = 0.18435$.

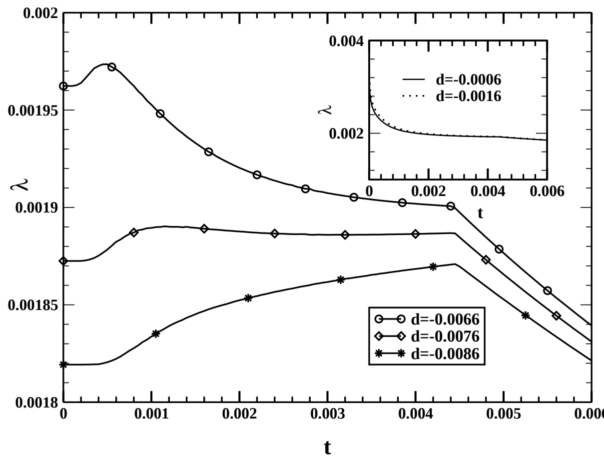

Figure 11. Plot of λ vs. t for different values of $d = -0.0066$, -0.0076, -0.0086 with fixed values of $u = 0.01$, $v = 0.0035$, $g_1 = 0.18435$. The inset shows the same plot for $d = -0.0006$, -0.0016.

a second electron at the site to form a localized Cooper pair is not favourable energetically due to Coulomb repulsion. But for the bare f-level close to the Fermi level thermal fluctuations deplete its occupancy, because of which forming a pair does not cost in energy, which enhances z_2. As expected, the superconducting transition temperature t_c remains the same for all the parameters. The effect of increasing the strength of hybridization from $v = 0.0035$ to 0.005 on z_1 and z_2 for $d = -0.0066$ are shown in figures 9 and 10 respectively. On increasing v, the SC transition temperature t_c and the magnitude of z_1 decrease, while that of z_2 increases, as can be seen from figures 9 and 10. As can be seen from eqs (8) and (10), when all the quantities are expressed in dimensionless form, a factor of

$N(0)\omega_D$ remains multiplied outside the integral which is the number of states in the energy range of ω_D. This quantity will take different values in eq. (8) compared to that in eq. (10) because the widths of the conduction band and f-levels are different. Accordingly the values of dimensionless $\tilde{N}(0)$ are chosen to be 30 and 4 for eqs (8) and (10) respectively. In order to estimate the hybridization gap (if it exists) and find its temperature dependence we calculate the parameter $\lambda(T)$ from eq. (11). Its behaviour for different values of the position of the bare f-level are shown in figure 11. It is interesting to note that there is a qualitative difference in the temperature dependence of λ for the cases when the effective f-level d_1 lies above the Fermi level (inset in figure 11) from that when it lies below the Fermi level (figure 11).

As the position of the f-level is pushed to lower values below the Fermi level, $\lambda(T)$ decreases in magnitude but shows a linear increase with temperature up to t_c. When the superconductivity sets in at $t < t_c$ there is an abrupt suppression in the magnitude of the hybridization parameter $\lambda(T)$. This suppression is more when the bare f-level is deeper ($d = -0.0086$) within the Fermi sea. There is a second depression in $\lambda(T)$ at a much lower temperature. This latter temperature (t_k) corresponds to the formation of the hybridization gap. The choice of the parameters of the present model calculation are such that the superconducting transition takes place at a higher temperature, than the formation of the hybridization gap (t_k), i.e. $t_c > t_k$. On increasing the strength of the hybridization to sufficiently large values, it may be expected that one can realize the situation $t_k > t_c$; but at such values of v, superconductivity may get totally suppressed; as can be seen from the trend in figure 4. To verify this conjecture $\lambda(T)$ is calculated for $v = 0.005$ for two different values of the position of the bare f-level, i.e., $d = -0.0016$ and -0.0066; and the results are shown in figure 12. The qualitative difference in the behaviour of $\lambda(T)$ when d_1 lies above ($d = -0.0016$) or below ($d = -0.0066$) the Fermi level is further accentuated in figure 12.

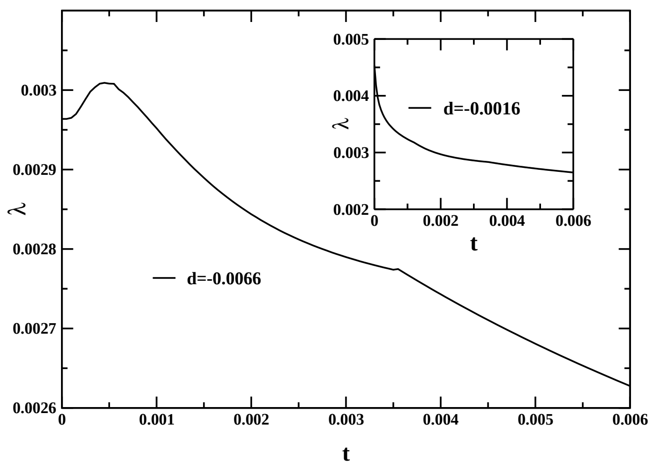

Figure 12. Plot of λ vs. temperature t for $d = -0.0066, u = 0.01, v = 0.005$ and $g_1 = 0.18435$. The inset shows the same plot for $d = -0.0016$.

It seems there is no perceptible effect on $\lambda(T)$ as the system makes the transition from the normal to the superconducting state with $\lambda(T)$ remaining more or less constant when d_1 is above the Fermi level. Furthermore, in this case on increasing v, $\lambda(T)$ undergoes an overall increase in its magnitude. In contrast, for d_1 below the Fermi level at the superconducting transition temperature t_c, there appears a kink in $\lambda(T)$, which gets reduced in magnitude below t_c; as compared to corresponding value in the absence of superconductivity. On increasing v, in this case there is an overall increase in $\lambda(T)$, in contrast to the case of the effective f-level lying above the Fermi level, where there was a decrease in $\lambda(T)$. Finally, there is the peaking of $\lambda(T)$ at t_k and its suppression at lower temperature. Somehow it seems that t_k does not change on increasing v in contradiction with the expectations. The hybridization parameter $\lambda(T)$ can be interpreted as the number of electrons having the characteristic of an admixture of c- and f-electrons. As can be seen from figures 11 and 12 this number which can be thought of as that of the heavy fermions is much smaller ($\sim$0.002) compared to that of the f-electrons ($\sim$1.0) amounting to about 0.2%. So, within this model the superconductivity is predominantly due to the conduction electrons and the contribution of the heavy fermions to SC is rather small, as is evident from figure 6.

Within the periodic Anderson model, there is the possibility for a real hybridization gap to develop in the electronic energy spectrum. If the gap lies at the Fermi level, then it will inhibit superconductivity, because the density of states at the Fermi level will become zero. Consequently, for the numerical calculations the parameters of the model are so chosen that superconductivity appears at higher transition temperature compared to the temperature at which the hybridization gap may appear.

To visualize the interplay between the superconductivity and the hybridization gaps, the density of states (DOS) is plotted as a function of frequency (energy) for the heavy fermion system, which is shown in figure 13 for different values of

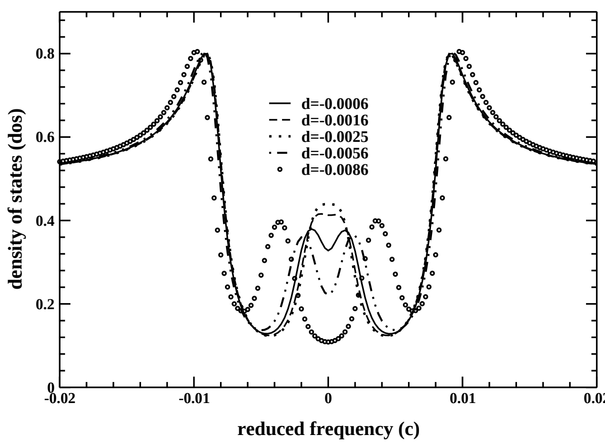

Figure 13. Plot of density of states (DOS) vs. reduced frequency (c) for different values of $d = -0.0006, -0.0016, -0.0025, -0.0056, -0.0086$ with fixed values of $u = 0.01, v = 0.0035$ and $e = 0.001$.

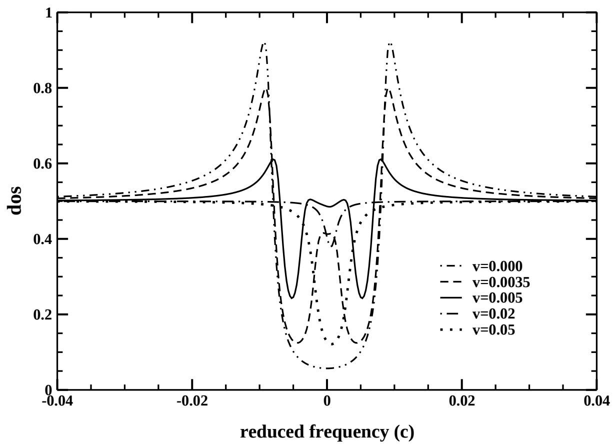

Figure 14. Plot of density of states (DOS) vs. reduced frequency (c) for different values of $v = -0.00, -0.0035, -0.005, -0.02, -0.05$ with fixed values of $d = -0.0016$, $u = 0.01$ and $e = 0.001$.

the position of the bare f-level. In plotting the density of states the values of the effective f-level (d_1) and the SC order parameter (z) at a particular temperature $t = 2 \times 10^{-3}$ are taken from figures 2 and 3 respectively. As can be seen from figure 13, for values of d for which d_1 lies above the Fermi level, the density of states peaks at the Fermi energy due to hybridization, while a well-developed SC gap of magnitude 0.02 appears in the DOS.

On the other hand, when the effective f-level d_1 lies below the Fermi level there appears a double peak structure at $\epsilon_{\rm F}$ in the DOS signifying the formation of the hybridization gap. It is worth pointing out that the magnitude of the DOS does not vanish either in the SC gap region or in the region of the hybridization gap. This behaviour is typical of a gap-less superconductor. The behaviour of the density of states for different values of the strength of the hybridization parameter v is shown in figure 14. As expected, when $v = 0$, only the SC gap exists, without any signature of the hybridization gap.

But even in this case the density of states does not vanish within the SC gap region. This non-vanishing of the DOS inside the gap region could be due to the presence of the f-level, which even though decoupled from the conduction band (because $v = 0$), still contributes to the density of states. By increasing the strength of the hybridization, the DOS first peaks at the Fermi level and then shows the signature for the formation of a double peak corresponding to the opening of the hybridization gap. It is clear from figures 13 and 14, that the DOS at the Fermi level $N(0)$ takes different values for different bare f-level positions as well as for different strengths of hybridization. Under these conditions the HFS is predominantly a metallic one. Furthermore, since this quantity $N(0)$ is multiplied to the strength of the superconducting interaction V_0 to give the dimensionless coupling constant g_1, the calculation of the temperature dependence of the SC order parameter z using a constant value for g_1 implies that V_0 is varied to keep g_1 the same for all values of d and v in the present calculation.

5. Conclusions

In conclusion we shall summarize the salient features of the model under consideration for describing the superconductivity in the HFS and bring out the main results obtained in this calculation. The heavy fermion system is described by the periodic Anderson model, but the strong electronic correlation between the localized f-electrons is treated in the mean-field approximation. The superconductivity in the system is described by a BCS-like pairing Hamiltonian between the itinerant conduction electrons. Because of the mean-field approximation, there is the loss of strong correlation physics, but the advantage is that the reduced problem becomes exactly solvable and every aspect of the calculation becomes numerically tractable. The effect of the Coulomb correlation reduces to the renormalization of the position of the f-level with respect to Fermi level. This renormalized position acquires a temperature dependence through the occupation probability (n^{f}) of the f-electrons. It is further assumed that the system under consideration is nonmagnetic. In this model the f-electrons, through their hybridization with the conduction electrons, acquire some itineracy and are responsible for the heavy fermion behaviour. However, the pairing interaction being effective among the conduction electrons, the heavy fermions contribute only a small fraction to the superconductivity. This induced pairing among the f-electrons and the pairing in the admixture of f- and conduction electrons are also calculated and shown to contribute only a small percentage to the superconductivity. The most important result of this calculation comes from the fact that the SC order parameter and its temperature dependence are affected by the renormalized position of the f-level with respect to the Fermi level and the latter depends explicitly on the f-electron number (n^{f}) and therefore there is a need for the self-consistent determination of the temperature dependence of the SC order parameter and that of n^{f}.

Since the renormalized f-level depends on the position of the bare f-level (d) and the inter-atomic Coulomb repulsion (u) the two can always be adjusted such that d_1 is always close to the Fermi level. So the absolute values of u or that of d does not affect the results. However, it is shown that there is a qualitatively different nature of the temperature dependence of the superconducting order parameter depending on whether d_1 is above or below the Fermi level. There is also a strong dependence of the superconducting order parameter on the strength of the hybridization (v). At $v = 0$, the reduced SC order parameter $z(t)$ shows the standard BCS behaviour, because the presence of the f-level does not interfere with superconductivity in the absence of the hybridization. However, as v increases there is a suppression in $z(t)$ at low temperatures, indicating the possibility of the formation of a hybridization gap or a pseudo-gap. This suppression is more prominent when the renormalized f-level approaches the Fermi level from above. With further increase in the strength of the hybridization, the low temperature suppression of $z(t)$ increases to the extent that superconductivity shows the re-entrant behaviour and ultimately disappears completely. For these values of v for which superconductivity disappears, there appears a real hybridization gap which drives the HFS into an insulator. The other quantities related to superconductivity are the f-electron pairing (z_2) and the mixed pairing of the f- and conduction electrons (z_1). Their temperature dependences are also studied. Their overall contribution to superconductivity is rather small.

However, for d_1 above the Fermi level, the contribution of (z_2) at temperatures close to zero shoots up, becoming comparable to that of z. This may be an indication that a predominantly f-electron pairing may be responsible for the observed heavy fermion superconductivity. The dependence of (z_1) and (z_2) on the strength of the hybridization parameter v are similar to that of z when d_1 is above the Fermi level. On the other hand, when d_1 is below it shows that while (z_1) decreases (z_2) increases with increasing v. This again is an indication that hybridization favours the f-electron pairing and tends to push the system towards predominantly heavy fermion superconductors.

The next quantity that is calculated is the temperature dependence of the hybridization parameter $\lambda(t)$. This quantity, which is a measure of the number of heavy fermions in the system, also shows qualitatively different behaviour for d_1 above or below the Fermi level. In the former case λ remains constant at almost all temperatures, rising sharply close to zero temperature. The onset of superconductivity at and below t_c has no perceptible effect on the temperature dependence of $\lambda(t)$, when d_1 is above the Fermi level. On the other hand, when d_1 is below the Fermi level in the normal state as one approaches t_c, there is a linear rise in λ. At t_c there is a sharp suppression in λ, the suppression being larger as d_1 moves deeper into the Fermi sea of the conduction electrons. At low temperatures close to zero there is a peaking in $\lambda(t)$ followed by a dip which flattens when d_1 moves deeper into the Fermi sea. This dip at low temperatures may be the signature of the appearance of the hybridization gap. Thus the superconducting state as well as the formation of the hybridization gap tends to suppress the number of electrons with mixed, localized f- and itinerant conduction electron character. On increasing the strength of the hybridization there is an overall increase in $\lambda(t)$ at all temperatures both for d_1 above and below the Fermi level, while the qualitative nature of the temperature dependence remains unchanged. Finally, the quasi-particle density of states (DOS) is calculated, which shows the existence of a pseudo-gap across the Fermi level due to the appearance of superconductivity. The signature of formation of yet another pseudo-gap at the Fermi level due to the opening of a hybridization gap can also be seen when the renormalized f-level is below the Fermi level. When the f-level is above the Fermi level there appears a peak in the density of states at the Fermi level. Thus there is always a finite density of states at the Fermi level which confirms that the systems under consideration are metallic ones. The pseudo-gap behaviour of superconductivity mimics the gap-less superconductors even in the absence of magnetic impurities. This gap-less behaviour persists even when the strength of the hybridization is zero, a case where the f-level is decoupled from the conduction electrons so that hybridization peak or gap appears at the Fermi level.

The experimental observation of superconductivity in heavy fermion systems so far has focused its attention on the pairing of heavy quasi-particles. This investigation points out that there may be systems in the family of heavy fermion superconductors, in which the pairing takes place between the normal itinerant electrons rather than the heavy quasi-particles. The mechanisms of the pairing in the two cases could be different. For heavy quasi-particle pairing, the mechanism will be non-conventional, while for the itinerant electron pairing it could be the usual BCS phonon exchange mechanism. If such systems are found, they could be the candidates for the co-existence of superconductivity with two different pairing symmetries.

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