Coexistence of antiferromagnetism and superconductivity in the Anderson lattice

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Abstract
We study the interplay between antiferromagnetism and superconductivity
in a generalized infinite-U Anderson lattice, where both superconductivity
and antiferromagnetic order are introduced phenomenologically in mean
field theory. In a certain regime, a quantum phase transition is found
which is characterized by an abrupt expulsion of magnetic order by d-wave
superconductivity, as externally applied pressure increases. This transition
takes place when the d-wave superconducting critical temperature, T_c,
intercepts the magnetic critical temperature, T_m, under increasing pressure.
Calculations of the quasiparticle bands and density of states in the ordered
phases are presented. We calculate the optical conductivity $\sigma(\omega)$ in the clean
limit. It is shown that, when the temperature drops below T_m, a double peak
structure develops in $\sigma(\omega)$.

1. Introduction

It is a common feature of several strongly correlated electronic systems that the low temperature
ordered phases compete with each other. In particular, competition between antiferromagnetic
and superconducting orders is an important characteristic of heavy-fermion systems [1], which
is also shared by high-T_c materials [2] and low-dimensional systems [3]. The closeness of
the superconducting phase to the antiferromagnetic phase in heavy fermion compounds has
led to the conjecture that the attractive interaction leading to superconductivity is actually
mediated by a magnetic excitation [1], instead of the traditional phonon mechanism. Also,
the interplay between antiferromagnetism and superconductivity has been proposed to be
described by a $SO(5)$ symmetry breaking [4]. The complexity of these systems arises from
the interplay between Kondo screening of the local moments, the antiferromagnetic Ruderman–
Kittel–Kasuya–Yosida (RKKY) interaction between the local moments and superconducting
correlations between the heavy quasiparticles.

Heavy-fermion systems that exhibit both superconductivity and antiferromagnetism
exhibit ratios between the Néel temperature T_N and the superconducting critical temperature

T_c that can vary substantially (of the order of $T_N/T_c \sim 1$–100), with coexistence of both types of order below T_c. The coexistence of both types of order can be tuned by external parameters such as externally applied pressure or chemical pressure (involving changes in the stoichiometry) [1, 5]. Examples of heavy-fermion materials which exhibit antiferromagnetic and superconducting order at low temperature are URu_2Si_2 and $U_{0.97}Th_{0.03}Be_{13}$. It has recently been found that UPd_2Al_3 ($T_N = 14.3$ K and $T_c = 2$ K) and UNi_2Al_3 ($T_N = 4.5$ K and $T_c = 1.2$ K) show the coexistence of superconductivity and local moment antiferromagnetism [1, 6–9]. However, in the Ce-based heavy-fermions magnetism typically competes with superconductivity. In the prototype heavy-fermion system $Ce_xCu_2Si_2$ both coexistence and competition between d-wave superconductivity and magnetic order has been clearly observed in a small range of x values around $x \simeq 0.99$ pressure [5]. This system exhibits a magnetic 'A phase' at low temperature whose detailed nature is not yet known. Increasing pressure reduces the critical temperature T_A of the A phase. Recent studies [5, 10–12] of $CeCu_2Si_2$ samples near the stoichiometric composition have shown that a d-wave superconducting phase expels the magnetic 'A phase' when T_A approaches T_c under increasing pressure.

In general terms, the local moments due to the f-electrons are progressively quenched as the temperature is lowered. In dilute systems the picture is well understood as being due to Kondo screening by the conduction electrons. In dense systems, however, the picture is more involved. At low temperatures the local moments are not completely quenched. In U-based materials such as URu_2Si_2, UPt_3 or UPd_3, for instance, the remaining moments are quite small, of the order of 0.01–0.03 μ_B, but for other systems such as UPd_2Al_3 the local moment is quite large, of the order of 0.85 μ_B. The low temperature magnetic behaviour of Ce-based compounds such as $CeCu_2Si_2$ and $CeCu_{6-x}Au_x$ has been interpreted as being due to the vicinity to a quantum critical point [13] where the Néel temperature tends to zero. Two pictures arise, however [14]: in the first one the Kondo temperature is high (the moments are quenched at a finite temperature) and when the system approaches the quantum critical point there are no free moments (assuming that quenching is complete). Then the system has to order due to a Fermi surface instability of the spin density wave type. Another possible situation is one in which the moments are not completely quenched down to $T = 0$ and are free to orient themselves, leading to magnetism. In the case of $CeCu_{6-x}Au_x$ evidence has been recently found that the second picture seems to hold [14] but a small but finite Kondo temperature has been quoted for this material (see the second reference in [13]). On the other hand, the high value of the Kondo temperature for the $CeCu_2Si_2$ compound [5] indicates possibly that the first scenario should hold. Furthermore, recent experiments [15] with $CeRh_{1-x}Ir_xIn_5$ also reveal an unusual coexistence of magnetism and superconductivity. It appears that in this system the f-electrons are more band-like than localized. On the other hand, in UPd_2Al_3 it is the dual character of the 5f electrons that leads to the high value of the local moment in coexistence with the itinerant electrons and with the superconductivity [7].

On the theoretical side it is believed that the Anderson model and its extension to the lattice captures the basic physics of the heavy fermions [16]. In this model the conduction electrons, c, (usually regarded as free) hybridize with local states, f, where the electrons are strongly interacting in such a way that the Coulomb repulsion, U, between two f-electrons is the largest energy scale in the problem. Frequently the limit $U \rightarrow \infty$ is taken, implying that double occupancy is forbidden. The limit $U = \infty$ has been studied using the slave boson technique [17–19]. In particular, it has been shown that superconducting instabilities arise in the p and d-wave channels because of the effective RKKY interaction between the f-electrons [19, 20]. Recently, the magnetic and superconducting instabilities of the normal phase were studied in the random phase approximation (RPA) [21] by taking into account slave

boson fluctuations above the condensate. However, the competition/coexistence between both types of ordering was not considered.

In this work we consider the $U = \infty$ Anderson lattice model in the slave-boson approach. Because our aim is to study the interplay between magnetism and superconductivity, we explicitly introduce antiferromagnetic and superconducting couplings phenomenologically. The coupling constants are taken as independent even though they are related if the superconducting mechanism is mediated via the RKKY interaction. Using a mean field approach we study directly the ordered phases and determine regimes of coexistence or competition between the two ordered phases, depending on the parameters of the model.

In this work we will take the conduction electrons to be non-interacting but we should also mention that attempts to include interactions between the conduction electrons have been carried out [22, 23]. The inclusion of this more realistic interaction has been found to be required in some systems to attain a better understanding of the experimental results. We focus our attention on the coexistence of superconducting correlations and magnetic ordering in heavy fermions which, to our knowledge, has not yet been studied theoretically, despite the considerable recent experimental effort devoted to this subject.

2. Model Hamiltonian and quasiparticle spectrum

The microscopic description of superconductivity and magnetic order in the Anderson lattice model is a still unsolved problem. In the following we shall consider an effective Hamiltonian which originates from the $U = \infty$ Anderson model with two additional phenomenological terms: one where superconducting correlations are explicitly assumed between the local f-electrons (since it is believed that pairing occurs between heavy quasiparticles which, therefore, have essentially f-character) and another term where local spins are coupled antiferromagnetically. The infinite Coulomb repulsion between the f electrons is described within Coleman's slave-boson [18] technique with a condensation amplitude $\sqrt{z}$. The effective Hamiltonian is therefore

$$H^{\mathrm{MF}} = \sum_{k\sigma}(\epsilon_k - \mu)c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k\sigma}(\epsilon_{\mathrm{f}} - \mu)f_{k\sigma}^\dagger f_{k\sigma} + \sqrt{z}V\sum_{k\sigma}(f_{k\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger f_{k\sigma})$$
$$+ z\sum_k(\Delta_{\mathrm{f}}\eta_k f_{k\uparrow}^\dagger f_{-k,\downarrow}^\dagger + \Delta_{\mathrm{f}}^*\eta_k f_{-k,\downarrow}f_{k\uparrow}) - 2m\sum_{k\sigma}\sigma(f_{k\sigma}^\dagger f_{k-Q,\sigma} + f_{k\sigma}^\dagger f_{k+Q,\sigma})$$
$$+ (\epsilon_{\mathrm{f}} - \epsilon_0)(z-1)N_{\mathrm{s}} + \frac{2N_{\mathrm{s}}m^2}{J_{\mathrm{m}}} - \frac{N_{\mathrm{s}}|\Delta_{\mathrm{f}}|^2}{J_{\mathrm{f}}}. \tag{1}$$

The c and f operators refer to conduction and localized electrons and obey the usual anticommutation relations. For simplicity, the hybridization potential V is assumed to be momentum independent, ϵ_0 and ϵ_{f} denote the bare and renormalized f-level energies and N_{s} denotes the number of lattice sites.

Although it is known that conduction electrons provide an effective RKKY interaction between f electrons, we remark that the superconducting and magnetic order parameters in (1) *cannot* be *simultaneously* derived from a Hubbard–Stratonovich decoupling of a single RKKY term of the form $\tilde{J}_{ij}\vec{S}_i \cdot \vec{S}_j$, as discussed, for instance, in [24]. This is why we have phenomenologically introduced those terms.

In writing down the pairing term in (1) we have in mind that in the slave-boson formulation a slave-boson operator b_i is associated with every f_i operator to prevent double occupancy. Condensation of the slave bosons is described by the replacement $b_i \to \langle b_i \rangle = \langle b_i^\dagger \rangle = \sqrt{z}$, hence the factor z in the superconducting term of (1) [25, 26]. The superconducting order parameter is given by $\Delta_{\mathrm{f}} = \frac{zJ_{\mathrm{f}}}{N_{\mathrm{s}}}\sum_k \eta_k\langle f_{-k,\downarrow}f_{k\uparrow}\rangle$, where η_k denotes any of the possible pairing

symmetries $\eta_k^{(s)} = \cos k_x + \cos k_y$, $\eta_k^{(p,i)} = \sqrt{2} \sin k_i$ and $\eta_k^{(d)} = \cos k_x - \cos k_y$ for s, p and d waves, respectively. Here we consider two dimensions for simplicity of the calculations. We take a square lattice even though several heavy fermions have a complicated lattice structure since we want to capture the main features.

The magnetic order parameter is given by the mean field equation $m_i = J_m \langle f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\downarrow}^\dagger f_{i\downarrow} \rangle$ and $m_i = 2m \cos(\vec{r}_i \cdot \vec{Q})$, where $\vec{Q} = (\pi, \pi)$ is the antiferromagnetic ordering vector. We consider only commensurate antiferromagnetic correlations since it is particularly relevant to the systems referred to.

In the calculations we assume a simple dispersion for the conduction electrons, of the form $\epsilon_k = -2t \sum_{i=x,y} \cos k_i$. For a given particle density the chemical potential must be computed from the condition $n_c + n_f = n$. The mean field equations obtained from minimization of the free energy of Hamiltonian (1) are solved numerically. The solution gives the interplay between the boson condensation, the magnetization and superconducting pairing as a function of band-filling and of the various model parameters. Throughout this work we will consider only the case of d-wave pairing. The other two pairings give qualitatively similar results in most regimes, as stressed before for the case of no magnetism and only superconducting order [25]. In different regimes different pairing symmetries become the most stable one but the overall behaviour is similar. However we will get back to this point later. We will consider temperatures such that the slave bosons are condensed and therefore we quench the f-electron density fluctuations.

2.1. Magnetic non-superconducting phase

We begin by discussing the magnetic but non-superconducting phase of the model. A detailed study of the superconducting non-magnetic phases has been presented elsewhere [23, 25].

In order to diagonalize (1) for $J_f = 0$ we introduce a quasiparticle operator which is a linear combination of the operators forming the basis $(c_{k\sigma}^\dagger; c_{k+Q,\sigma}^\dagger; f_{k\sigma}^\dagger; f_{k+Q,\sigma}^\dagger)$. We write the Hamiltonian in this basis. The mean field equations are obtained varying the effective Hamiltonian in the usual way. Minimization of the free energy of (1) with respect to z gives

$$\epsilon_f - \epsilon_0 = -\frac{V}{2\sqrt{z}} \frac{1}{N_s} \sum_{k\sigma} (\langle f_{k\sigma}^\dagger c_{k\sigma} \rangle + \langle c_{k\sigma}^\dagger f_{k\sigma} \rangle). \tag{2}$$

The condition $n_f + z = 1$ is

$$z = 1 - \frac{1}{N_s} \sum_{k\sigma} \langle f_{k\sigma}^\dagger f_{k\sigma} \rangle, \tag{3}$$

and the chemical potential is related to the total particle density as

$$n = \frac{1}{N_s} \sum_{k\sigma} \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle + \frac{1}{N_s} \sum_{k\sigma} \langle f_{k\sigma}^\dagger f_{k\sigma} \rangle. \tag{4}$$

The magnetization is given by

$$m = \frac{J_m}{2N_s} \sum_{k\sigma} \sigma \langle f_{k\sigma}^\dagger f_{k-Q,\sigma} + f_{k\sigma}^\dagger f_{k+Q,\sigma} \rangle. \tag{5}$$

For the sake of comparison, we show in figure 1 the quasiparticle bands and the density of states for a situation where the magnetic order parameter is zero and nonzero, respectively. We see that, in addition to the hybridization gap, there is an additional gap due to the magnetic order. The magnetic order with momentum $\vec{Q}$ reduces the size of the Brillouin zone to a half of that of a non-magnetic system.
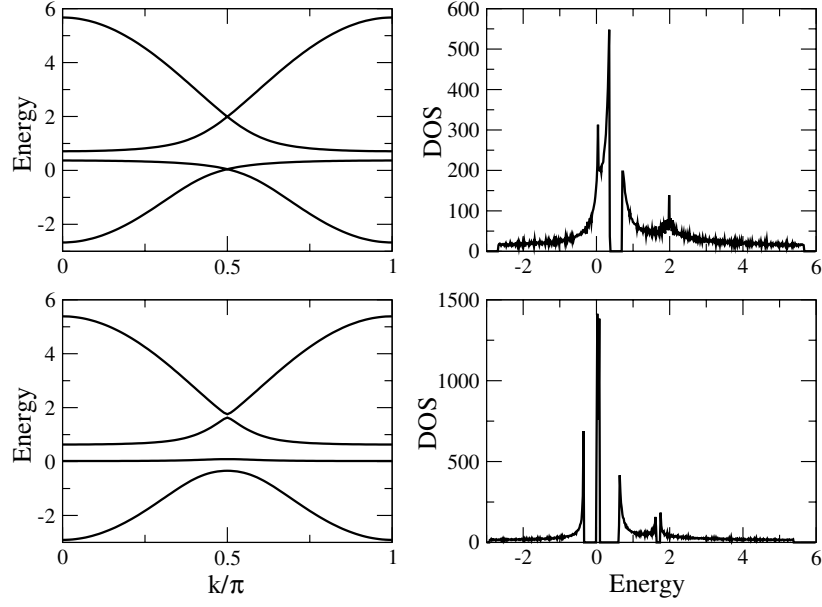
Figure 1. Quasiparticle bands and density of states for the magnetic coupling $J_m = 0$ in the top panels and $J_m = 0.9$ in the lower panels along the direction $k_x = k_y = k$. Model parameters are: $t = 1$, $n = 0.9$, $V = 1.0$ and $\epsilon_0 = -1.5$. The energies are measured with respect to the chemical potential.

2.2. Coexistence of antiferromagnetism and superconductivity

The Hamiltonian matrix H_k can be written in the basis

$$(c_{k\uparrow}, c_{k+Q,\uparrow}, f_{k,\uparrow}, f_{k+Q,\uparrow}, c^\dagger_{-k,\downarrow}, c^\dagger_{-k-Q,\downarrow}, f^\dagger_{-k,\downarrow}, f^\dagger_{-k-Q,\downarrow})$$

as

$$H_k = \begin{pmatrix} A_+ & D \\ D^\dagger & A_- \end{pmatrix}$$

where the matrices $A_\pm$ and D are given by

$$A_\pm = \begin{pmatrix} \pm\epsilon_k & 0 & \pm\sqrt{z}V & 0 \\ 0 & \pm\epsilon_{k+Q} & 0 & \pm\sqrt{z}V \\ \pm\sqrt{z}V & 0 & \pm\epsilon_f & -2m \\ 0 & \pm\sqrt{z}V & -2m & \pm\epsilon_f \end{pmatrix}$$

and

$$D = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & z\Delta_f\eta_k & 0 \\ 0 & 0 & 0 & z\Delta_f\eta_{k+Q} \end{pmatrix}.$$

The energies are measured with respect to the chemical potential. The eigenvectors of the matrix H_k are the Bogolubov operators expressed in the same basis.

Variation of the free energy with respect to z shows that (2) must now be replaced by

$$\epsilon_f - \epsilon_0 = -\frac{V}{2\sqrt{z}N_s}\sum_{\vec{k},\sigma}(\langle f^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma}\rangle + \langle c^\dagger_{\vec{k},\sigma} f_{\vec{k},\sigma}\rangle) - \frac{2N_s}{zJ_f}\Delta_f^2 \qquad (6)$$

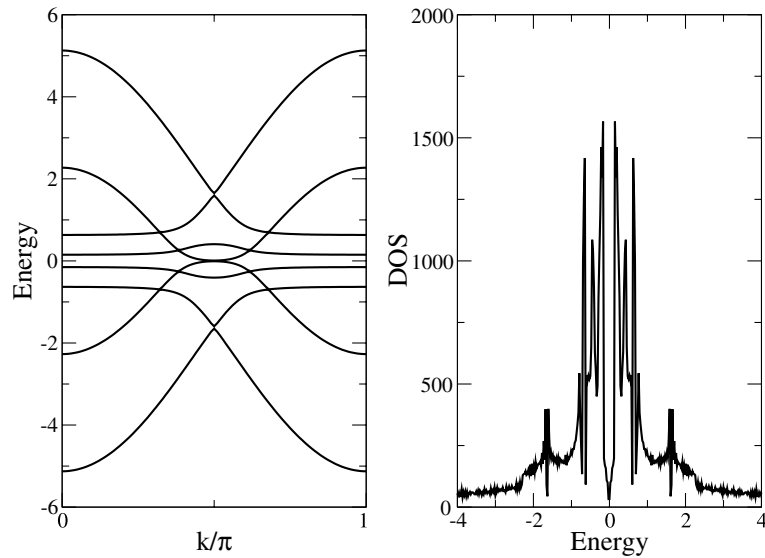while the other mean field equations remain unaltered.

Figure 2. Quasiparticle bands and density of states for the couplings $J_m = 0.9$, $J_f = -3$ for the Anderson model with magnetism and superconductivity. The other parameters are $n = 0.9$, $V = 0.6$, $\epsilon_0 = -1.5$ and the hopping $t = V/0.66$.

In figure 2 we show a typical quasiparticle band structure for the case where there is coexistence of magnetism and superconductivity. The quasiparticle bands are symmetric around the chemical potential due to the particle–hole structure of the Bogoliubov operators. Due to the superconducting order the spectrum is gapless.

3. Phase diagrams

The phase diagram of the model is quite rich due to the various correlations and order parameters considered. In this work we focus our attention on regimes where magnetism and superconductivity coexist or compete.

In figure 3 we plot the magnetization and the d-wave superconducting order parameter as functions of temperature for a typical case. The critical temperature for the antiferromagnetic order parameter m, T_m, is larger than the critical temperature, T_c, for d-wave superconductivity. At low temperatures the two phases coexist. While $\Delta_f \to 0$ the magnetization m is increasing and then m decreases to zero at T_m in the usual mean-field-like manner.

The left panel of figure 4 shows the order parameters m and Δ_f as functions of band filling at a fixed low temperature $T = 0.001$. For low to intermediate band fillings superconductivity exists. As the band filling increases, the superconductivity is less favourable while the magnetic order parameter appears, as expected, since the magnetic order is more favoured if the local electron density is higher. The value of Δ_f vanishes at low densities because the f-level occupancy also becomes small in that limit ($z \to 1$, $n_f \to 0$) and Cooper pairing occurs only between the f-electrons in the model considered. In the high density limit, Δ_f also tends to zero because the f-level occupancy is higher, approaching 1, and freezing of the charge fluctuations occurs due to the infinite on-site repulsion. Furthermore, a comparison with earlier results [25], where magnetic order was not considered, shows that magnetic order lowers the maximum value of the band filling for which $\Delta_f \neq 0$, indicating that the two effects compete with each other. At smaller band fillings incommensurate antiferromagnetic order also stabilizes.
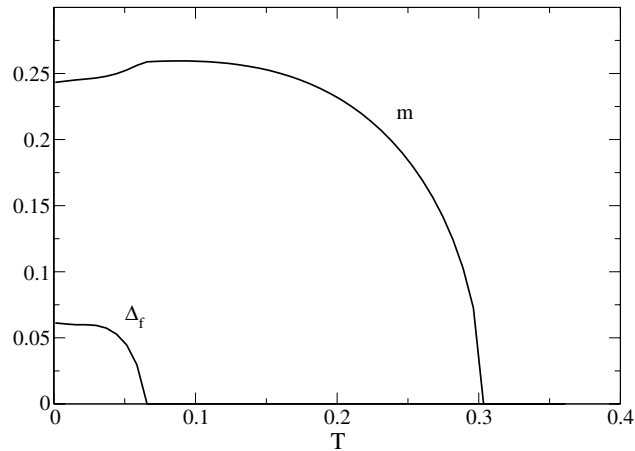
Figure 3. Magnetization and d-wave superconducting order parameters as functions of temperature for $n = 1$, $t = 1$, $\epsilon_0 = -1.5$, $J_f = -3$, $J_m = 0.9$, $V = 0.66$.
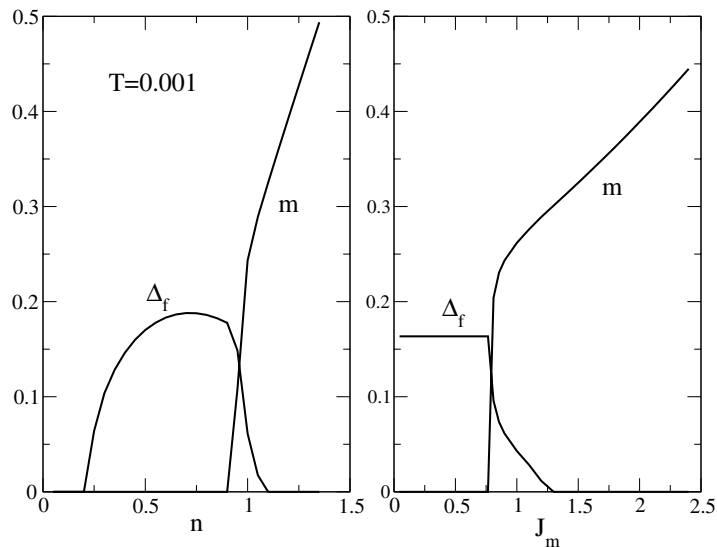

Figure 4. Magnetization and superconducting order parameters as functions of band-filling n in the left panel and of J_m in the right panel at a low temperature $T = 0.001$. The other parameters are the same as in figure 3.

Indeed, it extends to lower band fillings as compared to the commensurate case. However, the superconducting order expels the incommensurate case as well and including both types of ordering the phase diagram is qualitatively similar for commensurate or incommensurate order if superconductivity is also allowed.

The behaviour of the order parameters against magnetic coupling, J_m, at low temperature is shown in the right panel of figure 4. Increasing J_m leads to a crossover from a region where $m = 0$ to a regime where m grows with J_m while Δ_f follows the opposite trend. Keeping J_m fixed and decreasing J_f leads to the opposite result where the superconductivity disappears in favour of magnetism.
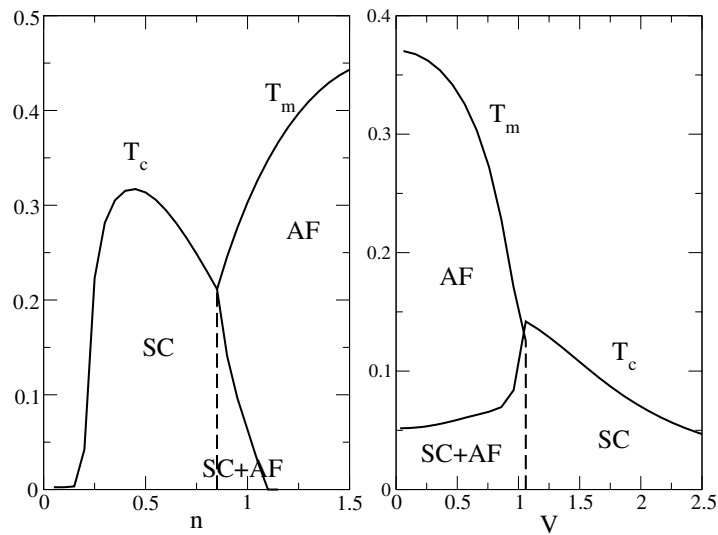
Figure 5. Critical temperatures T_c and T_m as functions of band filling, n and of V. The other parameters are the same as in figure 3. The antiferromagnetic (AF), superconducting (SC) and coexisting phases (SC + AF) are shown.

In figure 5 we plot the two critical temperatures as functions of the band filling and of the hybridization. The behaviour of the critical temperatures against density follows the same trend as in figure 4: for low n the superconducting temperature is higher while for higher densities $T_m > T_c$, indicating which phase is favoured as one lowers the temperature from the disordered high temperature phase. Lowering ϵ_0 or V has the tendency to increase f occupancy favouring magnetic order over superconducting order. At the point where the two temperatures cross the magnetic temperature falls abruptly to zero if the Cooper pairing symmetry is d-wave. This does not happen if the pairing symmetry is either extended s- or p-wave. In these cases there is no abrupt expulsion of the magnetization when the magnetic critical temperature becomes lower than the superconducting critical temperature and the phase where AF and SC coexist extends for smaller band-filling values and for larger values of the hybridization.

In the light of the experimental results, it is clearly interesting to compare qualitatively these results with the experimental phase diagrams, where either external pressure or chemical pressure are varied. Increasing pressure is expected to increase both hopping and hybridization amplitudes, while probably keeping V/t and other parameters approximately constant, to a first approximation [27]. In figure 6 we plot the mean field temperatures as functions of V for fixed ratio V/t. As pressure increases the magnetic critical temperature decreases and T_c increases. Once again at the point where the two temperatures cross the magnetic temperature falls abruptly to zero if the Cooper pairing symmetry is d-wave. This result, showing expulsion of a spin-density-wave by d-wave superconductivity but not in the case of the other symmetries, is very similar to that of a previous study [28] where the problem of local moment formation in a superconducting phase was addressed: increasing pressure causes expulsion of local moments by d-wave superconductivity. Therefore, such a phenomenon occurs either in a scenario of (unscreened or partially screened) ordered local moments or in a spin-density-wave scenario, where magnetic order appears as a Fermi surface instability.

The abrupt decrease of m as T_c crosses T_m signals a quantum phase transition that can be tuned using the external pressure as a parameter: as pressure is reduced (at zero T) the ground
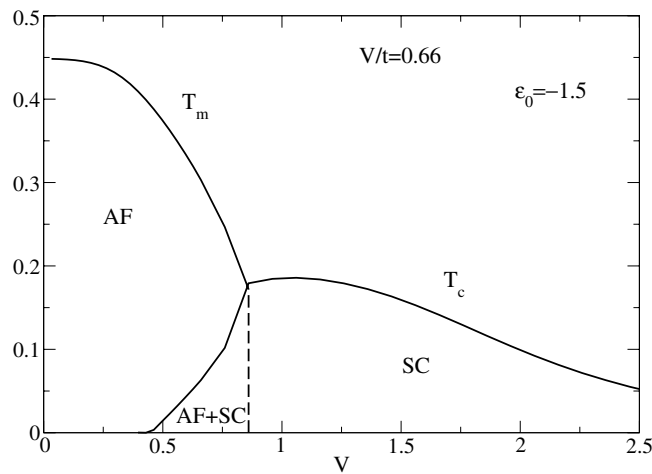
Figure 6. Critical temperatures T_c and T_m as functions of V, with fixed $V/t = 0.66$ for $\epsilon_0 = -1.5$. The other parameters are the same as in figure 3. The antiferromagnetic (AF), superconducting (SC) and coexisting phases (SC + AF) are shown

state of the system changes abruptly from nonmagnetic but superconducting to magnetic and superconducting at a critical value of V_c. The transition appears to be first order. We note that the same behaviour is found for the compound $CeCu_2Si_2$ [29].

Experimentally, most systems have quite large effective masses. Large mass enhancements are obtained when z is small ($n_f \to 1$). This is indeed observed in regimes where the AF order parameter is large but in these regimes superconductivity is absent. In figure 7 we show results for the quasiparticle bands and densities of states where a strong mass enhancement is seen for a large magnetization, in opposition to a situation where the magnetization is zero. In the calculations above, we have not been able to find regimes where there is a very large (say, larger than 200) mass enhancement. In the model considered, the appearance of superconductivity is restricted to the mixed valence regime. In this situation we do not expect very large densities of states at the chemical potential. In a more realistic approach U is large but finite and larger band fillings are allowed ($0 \leqslant n_f \leqslant 2$). We expect, therefore, that in this regime we might find large effective masses together with superconducting and magnetic order. The restriction to the mixed valence regime is a consequence of the slave-boson approach [30]. In this method the chemical potential is always pinned to the lowest quasiparticle band, the density is always smaller than one and the superconductivity only appears in the intermediate valence regime with moderate effective masses [31]. Nevertheless, our results reproduce qualitatively well the experimental phase diagrams and the competition between the d-wave superconducting and magnetic phases, such as that observed, for instance, in $CeCu_2Si_2$.

Model (1) is an effective Hamiltonian for the interacting c and f particles. Since the quasiparticles are heavy close to the top of the lowest band, as evidenced by the high values of the specific heat jump, we have modelled the superconducting interaction as taking place between the local f electrons, as usual. One may wonder, however, at the effect of adding a pairing term, with coupling constant J_c, between the c-electrons, since these are present at low energies close to the chemical potential. Considering a pairing term in the Hamiltonian in the standard way, with amplitude Δ_c, we can solve the mean field equations as before. The effect of this added term is shown in figure 8. In general, the hybridization exchanges electrons between the c and the f levels. Due to the restriction on level occupancy due to the infinite
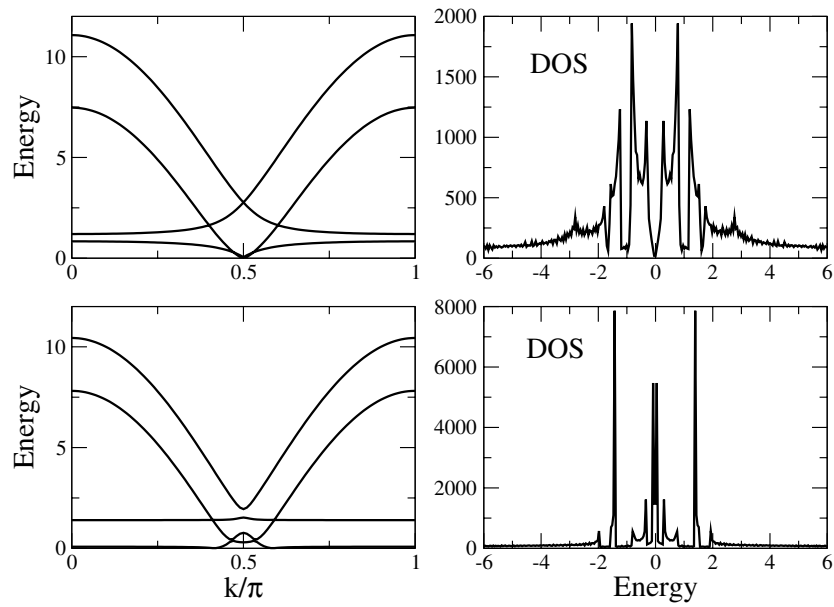
Figure 7. Top panels: quasiparticle bands and density of states for the set of parameters $n = 1$, $V = 1.5$, $t = V/0.66$, $\epsilon_0 = -1.5$, $J_f = -3$ and $J_m = 0.9$. For this set of parameters the system is in a phase where $\Delta_f = 0.108$, $m = 0$ and $z = 0.745$. Lower panels: quasiparticle bands and density of states for the set of parameters $n = 1.6$, $V = 1.5$, $t = V/0.66$, $\epsilon_0 = -1.5$, $J_f = -3$ and $J_m = 0.9$. For this set of parameters the system is in a phase where $\Delta_f = 0$, $m = 0.412$ and $z = 0.153$.
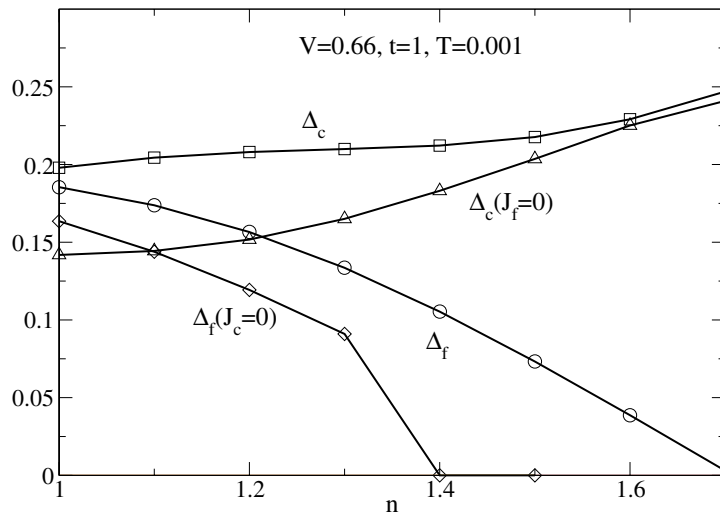

Figure 8. Superconducting order parameters Δ_f and Δ_c (see the text) as functions of band filling n at a low temperature $T = 0.001$ where we also include a c-electron pairing. The other parameters are the same as in figure 3.

U repulsion, for a fixed V as the density increases the number of f-electrons decreases and the superconductivity is destroyed, as discussed above. However, if the c electrons pair then

the order parameter Δ_c increases. As a consequence in figure 8 we see that, as the density increases, the ordering in the c-electrons increases. Actually, if we consider both types of pairing then the pairing in the f-electrons extends to higher densities. So in that sense adding the pairing between the c-electrons favours superconductivity at higher densities. However, we have found that the addition of this type of pairing inhibits the magnetism in the f-electrons probably due to the greater stability in the pairing channel.

We remark, however, that, had we written a BCS pairing term only among the c-electrons in the Hamiltonian (1), the resulting phase diagram would be quite different: the superconducting temperature would be maximum at zero hybridization and rapidly decrease with increasing V. This is easily understood because increasing V makes c-electrons heavier, hence reducing their pairing amplitude. Clearly this is the opposite trend to that found experimentally in the phase diagrams as a function of pressure where, at low hybridizations, superconductivity is absent, giving way to the magnetic order. Even if we do not include the possibility of magnetic order then it was shown before [25] that, for small values of the hybridization, the superconducting critical temperature is an increasing function of pressure. On the other hand, by having chosen a pairing interaction between f-electrons, we obtained increasing T_c since the f-electrons become more mobile upon increasing V. Therefore it is justified to consider only a pairing term between the heavy f-electrons.

4. Optical and dynamic conductivity

The study of the particle–hole excitations of a system can be probed by studying the finite frequency conductivity. Studies of the Anderson lattice have been carried out previously [17, 32] in the disordered phases and experimental results for the heavy fermions have been reviewed in [33]. In traditional superconductors the optical conductivity clearly shows a threshold at twice the gap energy [34, 35]. Since the dc conductivity of a perfect lattice is infinite, most studies are carried out taking into account scattering off impurities [36] considering moderate scattering up to the dirty limit [35, 36]. In this work we will study the optical conductivity in the clean limit and we shall study its behaviour in the ordered phases as well.

The real part of the dynamic conductivity is given by

$$\sigma_{\alpha\beta}(\vec{q}, \omega) = \frac{1 - e^{-\beta\omega}}{2\omega V} \int_{-\infty}^{\infty} dt \, e^{i\omega t} \langle j_\alpha^\dagger(\vec{q}, t) j_\beta(\vec{q}, 0)\rangle. \tag{7}$$

Writing the trace, inserting a decomposition of the identity in terms of the exact many-body energy states and integrating over time we obtain

$$\sigma_{\alpha\beta}(\vec{q}, \omega) = \frac{1 - e^{-\beta\omega}}{2\omega V} 2\pi \sum_{n,m} \frac{e^{-\beta E_n}}{Z} \delta(\omega + E_n - E_m)\langle n|j_\alpha^\dagger(\vec{q})|m\rangle\langle m|j_\beta(\vec{q})|n\rangle. \tag{8}$$

Consider now $\alpha = \beta$ and $\vec{q} = 0$. The $\alpha = x, y$ component of the current operator can be written as

$$j_\alpha = -it \sum_{\vec{k},\sigma} (\vec{\chi}_{\vec{k}})_\alpha c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} \tag{9}$$

where $\vec{\chi}_{\vec{k}} = \sum_{\vec{\delta}} \vec{\delta} e^{-i\vec{k}\cdot\vec{\delta}}$, where σ is the spin component. Writing the electronic operators in terms of the Bogolubov operators it is straightforward to calculate the matrix elements of the current operator.

We can also calculate the finite-momentum and finite-frequency conductivity $\sigma_{xx}(\vec{q}, \omega)$. Starting from equation (8) and taking similar steps to those followed for the calculation of the optical conductivity it is easy to calculate the dynamical conductivity.
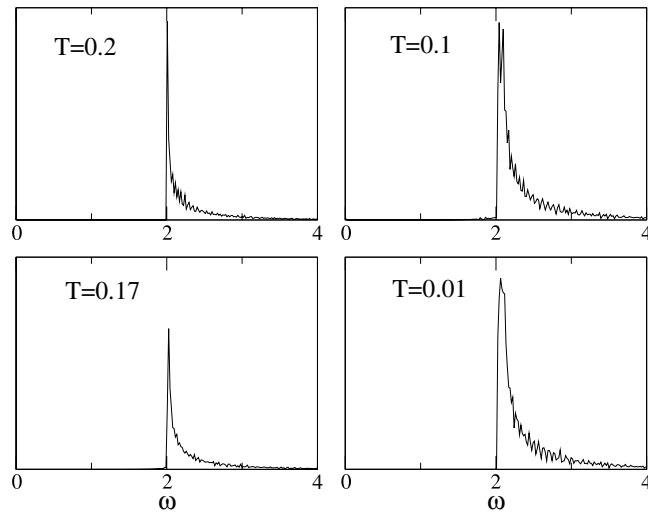
Figure 9. Optical conductivity (in arbitrary units) at several temperatures. $n = 1$, $V = 1.2$, $t = V/0.66$, $\epsilon_0 = -1.5$, $J_f = -3$ and $J_m = 0.9$. For these parameters the system is superconducting at low temperatures and has no magnetization.
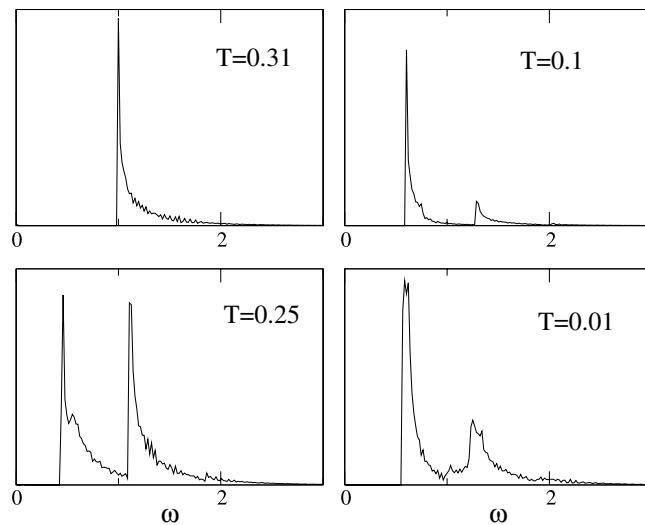

Figure 10. Optical conductivity (in arbitrary units) at several temperatures. $n = 1$, $V = 0.7$, $t = V/0.66$, $\epsilon_0 = -1.5$, $J_f = -3$ and $J_m = 0.9$. For the parameters chosen magnetism and superconductivity coexist at low temperatures.

In figures 9 and 10 we show the optical conductivity in the clean limit for two typical cases. Figure 9 refers to a regime where there is superconductivity but no magnetization at low temperature. Figure 10 refers to a regime where there is coexistence of superconductivity and antiferromagnetism at low temperature.

The experimental study of the optical conductivity, over a large range of frequencies, of some heavy-fermion systems has only recently become available [37, 38]. In [38] it was found that effective mass m^* of the quasiparticles increased about 50 times when the temperature
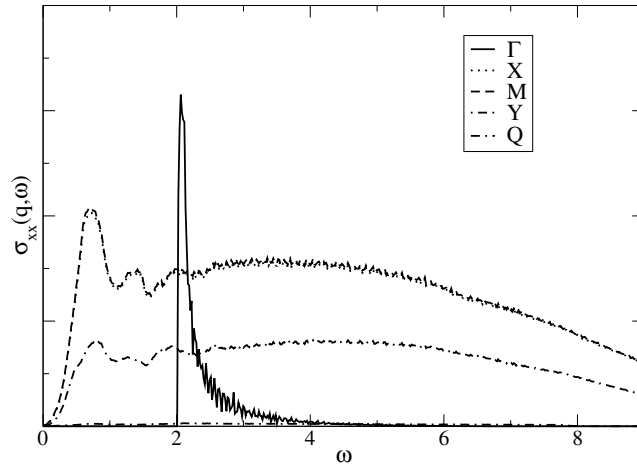
Figure 11. Finite-momentum and finite-frequency conductivity at several points in the Brillouin zone for a set of parameters such that the system is superconducting ($\Gamma = (0, 0)$, $X = (\pi, 0)$, $M = (\pi, \pi)$, $Y = (0, \pi)$, $Q = (\pi/2, \pi/2)$). The temperature is $T = 0.01$ and $V = 1.2$. The results for the Γ point, $\vec{q} = 0$, are multiplied by 1000.

decreases below the Néel temperature. Furthermore, the authors found for $T < T_N$ that a two-peak structure developed at finite frequencies. At temperatures higher than T_N the $\sigma(\omega)$ presents a single peak, separated from the Drude weight by a finite gap (if disorder is included the Drude peak broadens to finite energies). When the temperature drops below T_N a second peak, respecting the magnetic gap, shows up in $\sigma(\omega)$ at lower, but finite, energies. The features reproduced by our calculation are in qualitative agreement with the data presented in [38]. Also they are in qualitative agreement with the results of [39]. Note, however, that our model is not appropriate to describe this material since one needs to take into account the dual nature of the f-electrons, which is not included in our model. This shows that the results obtained are qualitative general trends that are captured by our simplified model.

In order to preserve momentum the optical conductivity probes the transitions between different bands coupled by the current operator. If we allow that momentum is interchanged then the dynamic conductivity also probes excitations along the same band in addition to across bands. In figures 11–13 we present the dynamic conductivity for different points in the Brillouin zone in three typical situations. In figure 11 the set of parameters and temperature are such that the system is superconducting, in figure 12 the system is both superconducting and magnetic, and in figure 13 the system is only magnetic. The gap structure evident in the optical conductivity ($\vec{q} = 0$) is now absent because low energy excitations are, in general, allowed since there is coupling between states in the same band. In the superconducting case (but not magnetic) the dynamic conductivity extends to zero frequency but vanishes in this limit due to the energy dispersion of the d-wave symmetry. If there is coexistence of superconductivity and magnetism then the same structure appears with the double-peak feature, characteristic of the magnetic phase, enhanced, as observed in the optical conductivity. If the superconducting order parameter is zero then the dynamic conductivity is finite at zero energy.

5. Summary

The interplay between magnetic correlations, the Kondo effect and superconducting correlations in heavy fermion systems is a difficult problem to solve. While previous
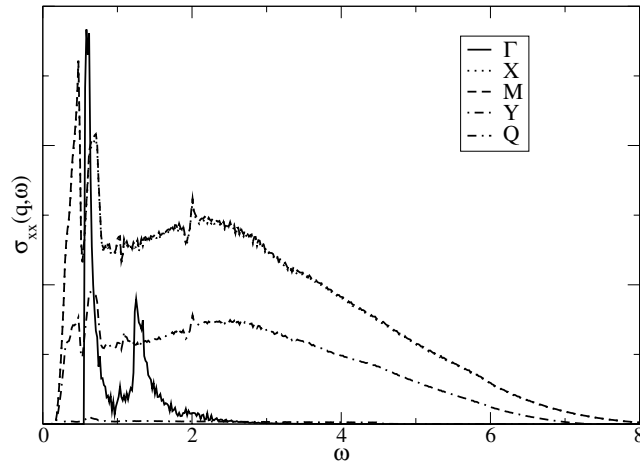
Figure 12. Finite-momentum and finite-frequency conductivity at several points in the Brillouin zone for a set of parameters such that the system is superconducting and magnetic. The temperature is $T = 0.01$ and $V = 0.7$. The results for the Γ point, $\vec{q} = 0$, are multiplied by 1000.
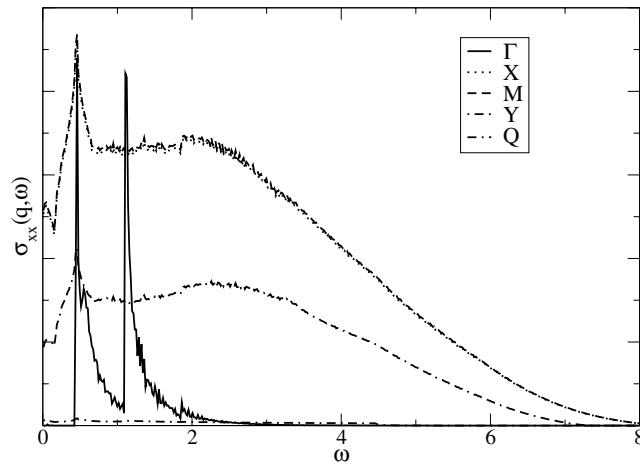

Figure 13. Finite-momentum and finite-frequency conductivity at several points in the Brillouin zone for a set of parameters such that the system is magnetic. The temperature is $T = 0.25$ and $V = 0.7$. The results for the Γ point, $\vec{q} = 0$, are multiplied by 1000.

studies on the $U = \infty$ Anderson lattice have identified the instabilities towards magnetic or superconducting order by taking into account the slave-boson fluctuations, the description of the ordered phases has not previously been carried out. In this work we have phenomenologically studied the interplay between the superconducting and antiferromagnetic ordered phases by studying their dependence on the model parameters. We have found that Cooper pairing symmetry plays an important role in determining the regimes of either coexistence or competition between superconductivity and antiferromagnetism: indeed, we have found that d-wave superconductivity coexists with antiferromagnetic order but the former expels the latter abruptly as the hybridization between the f-level and the conduction electrons increases. We also found that the f-level occupancy affects the two types of order in different ways: higher

occupancy favours antiferromagnetism while a lower occupancy favours superconductivity. Hence, the quasiparticle mass enhancement relative to the bare electron was found not to exceed a few tens in the superconducting phase. The optical conductivity has also been computed, reflecting the band structure of the ordered phases.

Acknowledgments

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