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Eliashberg equations in strong-correlation systems

L Puig-Puig, F López-Aguilar and J Costa-Quintana

Departament de Física, Grup d'Electromagnetisme, Universitat Autònoma de Barcelona, Bellaterra, E-08193 Barcelona, Spain

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Abstract. Eliashberg equations with a pair coupling potential constructed from screened fermion–fermion interactions arising from the strong-correlation energy U are solved to obtain the superconducting gap, the quasiparticle density of states in the superconducting state, and the transition temperature as a function of the band parameters in strongly correlated electron materials. This analysis allows us to establish the conditions of the electronic structure for obtaining coupling and superconductivity in these materials.

In the last few years, a new current of interest has risen in solving the Eliashberg equations in strongly correlated systems considering coupling potentials arising from screened fermion–fermion interactions [1–7]. This is, perhaps, due to the fact that theorists are consolidating the idea that the heavy-fermion systems and some high-T_c superconductors are strongly correlated materials whose pair coupling potentials, if present, are produced without intervening phonons at least in a fundamental way [1–10]. An open question is whether non-retarded potentials can explain these non-phononic superconductivities just considering the Bardeen–Cooper–Schrieffer (BCS) scheme and introducing van Hove singularities in the density of states (DOS) near to E_F [8–10], or whether it is necessary to consider dynamic potentials in order to reconcile theory to experiments. The previous analysis [7, 11, 12] leads us to think that strong-coupling equations are most appropriate in both superconducting cuprates and heavy fermions. The main point is to decide what kind of pair potential and what shape of the DOS in the vicinity of E_F should be included into the strong-coupling superconductivity equations. One possibility is to use fermion–fermion interactions from the random-phase approximation (RPA) plus the electron–hole ladder approximation (EHLA), and a DOS of the normal state of the strongly correlated materials which can be fitted by means of two Lorentzian curves, one each side of E_F, split by an energy 2λ and of widths Λ, which characterizes the electronic structure of these materials. In the case of the heavy-fermion systems the widths are much smaller than those of the d materials. Our purposes in this paper are (i) to consider an effective interaction similar to that considered in some recent literature [4, 13], including a bare polarization which we have used in several electronic structure calculations [14, 15] and that has given reasonable agreement with experimental results in other strongly correlated systems and (ii) to include this effective interaction in Eliashberg-like equations, for different values of the parameters of their electronic structures.

We start from a first-order approximation of the finite-temperature self-energies in the superconducting state corresponding to fermions and pairs [16] without considering vertex effects. In 1985 Sham [17] analysed these vertex effects in some plasmon-mediated

superconductivities and established that they can have quantitative influence. However, according to recent literature [18], these vertex effects can have importance in the cases of Hubbard systems with smaller Coulomb correlation energies and/or larger bandwidths than those considered in this paper. These 'normal' and 'pairing' self-energies can be written as

$$S(p, ip_n) = -\frac{1}{\beta}\sum_{q}\sum_{iq_n} V_{\text{eff}}(iq_n)G(p+q, ip_n + iq_n) \tag{1}$$

$$W(p, ip_n) = -\frac{1}{\beta}\sum_{q}\sum_{iq_n} V_{\text{eff}}(iq_n)F(p+q, ip_n + iq_n) \tag{2}$$

where V_{eff} is the effective pair interaction which will be commented on below and F and G correspond to the dressed correlation functions of the strong-coupling superconductivity, their expressions being

$$F(p) = \frac{-W(p)}{[ip_n Z(p)]^2 - [\xi(p)^2 + W(p)^2]} \tag{3}$$

$$G(p) = \frac{ip_n Z(p) + \xi(p)}{[ip_n Z(p)]^2 - [\xi(p)^2 + W(p)^2]} \tag{4}$$

where $W(p)$ is the self-energy for coupled pairs, and $Z(p)$ is defined from the 'normal' self-energy by

$$S(p) = S_{\text{sim}}(p) + ip_n\left[1 - Z(p)\right] \tag{5}$$

where $(p) = (\boldsymbol{p}, ip_n)$, and $S_{\text{sim}}(p)$ is the symmetric part of the self-energy for fermions, $S(p)$. A point with sufficient consensus is that in the strong-coupling limits, the Eliashberg equations applied to systems with short-ranged interactions can be treated considering the polarization and the effective interaction without $\boldsymbol{k}$-dependence [1–3, 14, 17], especially when one attempts to analyse the evolution of the W-function versus T, and the evolution of T_c with the band parameters, within the strong-coupling scheme and an s-wave character for the superconducting gap. In high-T_c superconductors there is, at the present time, a strong controversy [19, 20] about whether this orbital character is s or d. The d-wave treatment requires the introduction of $\boldsymbol{k}$-dependence in both the polarization and the pair potential. However, our study is addressed toward the strongly correlated systems in general, and our aim for this work is to analyse the possibility of an isotropic superconducting gap. Therefore, we determine the effective interaction $V_{\text{eff}}(iq_n)$ considering polarization functions averaged with respect to the $\boldsymbol{q}$ momenta of the first Brillouin zone [2, 3]. We consider the bare polarization function used in previous papers [14]

$$\chi(\omega) = \sum_{l}\frac{2\beta_l n_l(1-n_l)}{\omega^2 - \beta_l^2} \tag{6}$$

where n_l is the ocupation of the l symmetry of the strongly correlated orbital, and $\beta_l = 2(\lambda_l - i\Lambda_l)$, $2\lambda_l$ and Λ_l being the splitting and width of the two Lorentzian curves of the DOS both sides of E_F (for more information about these parameters and the polarization χ, see [14]).

Obviously, the ingredients of the model described in this paper are only compatible with the scenario proposed by the Hubbard Hamiltonian, which is clearly accepted both in heavy-fermion and high-T_c superconductors (see for instance [2–7, 13, 21]. This is an unquestionable assertion in the heavy-fermion systems, but it could be more doubtful in high-T_c superconductors, particularly if one considers that the pairing occurs between holes belonging to oxygen atoms. However, there is a tendency to think that even the p holes of oxygen atoms can be treated within the Hubbard Hamiltonian scheme, since the

Coulomb correlation energy for these p states is estimated between 4 and 8 eV [21]. In the strongly correlated superconductors the occupation ratio of the strongly correlated orbital has a large influence on the coupling, the existence of superconductivity, and its transition temperature. The RPA series in the effective interaction is dominant in systems with a sufficiently large number of interacting particles and the electron–hole ladder diagrams can produce significative effects for the cases with a small number of particles (or holes). Both series are complementary and non-redundant (except their first term), and therefore the effective interaction obtained as the sum of these two (RPA plus EHLA) effective interactions can be equally valid for any value of the occupation ratio of the strongly correlated orbital.

Considering the response function (6), the RPA and the EHLA effective interactions can be written as

$$V_{\mathrm{RPA}}(\omega) = U\,[1 - U\chi(\omega)]^{-1}$$
$$V_{\mathrm{EHLA}}(\omega) = U\,[1 + U\chi(\omega)]^{-1}$$

and the sum of both effective interactions can be expressed by means of the following general form:

$$V_{\mathrm{eff}}(\omega) = V_{\mathrm{RPA}}(\omega) + V_{\mathrm{EHLA}}(\omega) - U = U + U\sum_{k}\frac{f_k(\omega)}{\omega^2 - \Omega_k^2} \tag{7}$$

where $f_k(\omega)$ are functions without poles in the complex plane. When these functions are constant, they can be understood as the strengths of the k-oscillators which correspond to the coupling of the k intermediating equivalent bosons whose characteristic is the corresponding pole Ω_k. Expressions for both f_k and Ω_k can be deduced using an equivalent formulation given in [14], and depend on the number of active l-symmetries as well as on their band parameters. In this paper we consider a simplified case of effective interaction that can be illustrative, which is to consider the RPA plus the electron–hole ladder approximation [5, 13, 14] with a bare polarization (6) and a single orbital symmetry. Then, the resulting effective interaction can be written as

$$V_{\mathrm{eff}}(\omega) = U + U\frac{\Omega_1^2 - \beta^2}{\omega^2 - \Omega_1^2} + U\frac{\Omega_2^2 - \beta^2}{\omega^2 - \Omega_2^2} \tag{8}$$

where

$$\Omega_1^2 = \beta^2 + 4Un(1-n)\beta \tag{9}$$
$$\Omega_2^2 = \beta^2 - 4Un(1-n)\beta \tag{10}$$

with $\beta = 2(\lambda - \mathrm{i}\Lambda)$, and 2λ (Λ) stands for the splitting (width) of the two Lorentzian curves corresponding to the only strongly correlated orbital considered in this case. In addition, in the calculation carried out in this paper λ is less than $2Un(1-n)$ (i.e. we consider a not too wide band arising from the strongly correlated orbital), and in these conditions the term corresponding to the second pole (Ω_2) of (8) has a negligible influence on the effective interaction within the energy interval where it is attractive. Then, for the sake of simplicity in the calculation, we have considered as $V_{\mathrm{eff}}(\omega)$ a function of the type (7) with only one pole Ω considered as input parameter and with a strength $f(\omega) = \Omega_1^2 - \beta^2$.

In order to solve the self-energy equations, we consider the Lehmann representation of the correlation functions F and G

$$G(\boldsymbol{p}, \mathrm{i}p_n) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{2\pi}\frac{[-2\mathrm{Im}G_{\mathrm{ret}}(\boldsymbol{p}, \omega')]}{\mathrm{i}p_n - \omega'} \tag{11}$$

$$F(\boldsymbol{p}, \mathrm{i}p_n) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{2\pi}\frac{[-2\mathrm{Im}F_{\mathrm{ret}}(\boldsymbol{p}, \omega')]}{\mathrm{i}p_n - \omega'}. \tag{12}$$

After straightforward manipulations of (1) and (2), we obtain in the real frequency axis

$$W(\omega) = \int_{-\infty}^{\infty} d\omega' K(\omega, \omega') \mathrm{Im} \int_{-\infty}^{\infty} \frac{-N(x)W(\omega')}{(\omega' + i\delta)^2 Z(\omega')^2 - x^2 - W(\omega')^2} dx \tag{13}$$

$$S(\omega) = -\int_{-\infty}^{\infty} d\omega' K(\omega, \omega') \mathrm{Im} \int_{-\infty}^{\infty} \frac{N(x)\left[(\omega' + i\delta)Z(\omega') + x\right]}{(\omega' + i\delta)^2 Z(\omega')^2 - x^2 - W(\omega')^2} dx \tag{14}$$

where $K(\omega, \omega')$ is an intermediate function which contains the residues of the poles of V_{eff}, G and F that appear when evaluating the iq_n sum. This function takes the form

$$K(\omega, \omega') = -\frac{1}{2\pi}\left(U \sum_k \frac{f_k(\Omega_k)}{2\Omega_k} \frac{n_B(\Omega_k)}{\omega + \Omega_k - \omega'} - V_{\mathrm{eff}}(\omega' - \omega) n_F(\omega')\right) \tag{15}$$

where Ω_k and $f_k(\Omega_k)$ are the plasmon poles and strengths, respectively, arising from the oscillators which compose the effective interaction $V_{\mathrm{eff}}(\omega)$. The DOS $N(x)$ stands for the quasiparticles (fermions) which constitute the pair. In order to perform the calculation of these Eliashberg equations, we also approximate this DOS to two Lorentzians (similar to that considered in [14]), and we solve these equations in the band-parameter space in order to determine the region where superconductivity is possible. Looking at the DOS of the f and/or d electrons of the symmetries located at E_F in the strongly correlated systems [15], one can accept the validity of this approximation. On the other hand, we do not consider a constant DOS, as in standard BCS theory, because the energy interval in which the $W(\omega)$ and $Z(\omega)$ functions have large variations is of some eV and in this interval the DOS of the strongly correlated systems can present large variations. In this point the analysis is different from that made in standard strong-coupling superconductors where $N(x)$ is considered as a constant, since in our case the above-mentioned energy interval can even become one order larger than that of the phonon-mediated superconductors.

Equations (13) and (14) are solved by means of a self-consistent process, considering for the first iteration the expressions for F and G of the BCS theory for the weak-coupling model, i.e. with $W(\omega) = \Delta_0$ for $|\omega| \leqslant \omega_0$ and $W(\omega) = 0$ otherwise, and $Z(\omega) = 1$; for successive iterations, we consider $W(\omega)$ and $Z(\omega)$ of the former iteration. This iterative process is carefully treated to obtain convergence. The final result of $\Delta(\omega) = W(\omega)/Z(\omega)$ converges either to a constant function $\Delta(\omega) \to 0$ or to a function whose typical shape can be seen in figure 1. In the former case, one should interpret that for these values of the electronic structure parameters, superconductivity is not possible. In the cases in which superconductivity is present (see figure 1), the curves of $\Delta(\omega)$ have three characteristic features: (i) $\Delta(\omega)$ is an approximately even function with respect to ω; (ii) in a frequency interval $-\omega_0 < \omega < \omega_0$, $\mathrm{Re}\,\Delta(\omega)$ is positive, for $|\omega| > \omega_0$, $\mathrm{Re}\,\Delta(\omega)$ is negative, and for $|\omega| > \omega_c$ tends asymptotically to a small negative and constant value; (iii) when increasing the temperature, $\mathrm{Re}\,\Delta(\omega)$ keeps its shape but decreases for all ω values. Obviously, T_c is defined as the temperature for which $\mathrm{Re}\,\Delta(\omega)$ tends to zero for all ω. Figure 2 shows the evolution of the DOS of the superconducting state with the temperature, which corresponds to the evolution of the gap $\Delta(\omega)$ of figure 1: the decrease of the gap with the temperature up to $T = T_c$ can also be seen in the density of quasiparticles represented in figure 2. The features displayed in figures 1 and 2 appear in all strong-coupling superconductors, although in our calculation the tunnelling (optical) superconducting gap defined by the condition $\Delta_t = \Delta(\omega = 0)$ ($\omega = \Delta(\omega)$) can be one order larger than that of the standard superconductors if one conveniently chooses the band parameters, above all U, Λ, and λ.

In figure 3, we give the regions on the λ, Λ space where coupling and superconductivity are possible for different values of Ω, maintaining U and n fixed. These regions are smaller

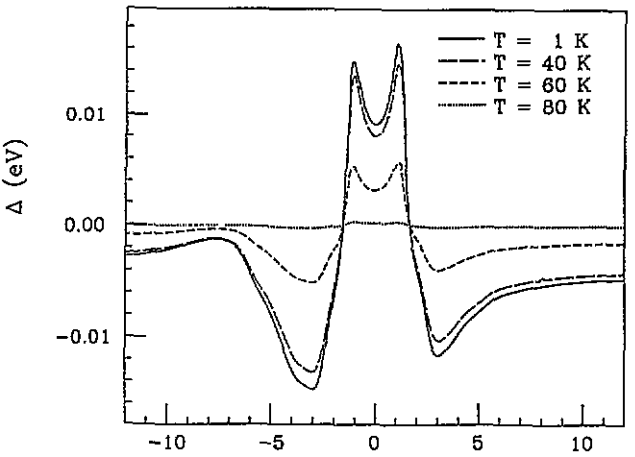

Figure 1. Superconductivity gap $\Delta(\omega)$ versus ω for different temperatures.

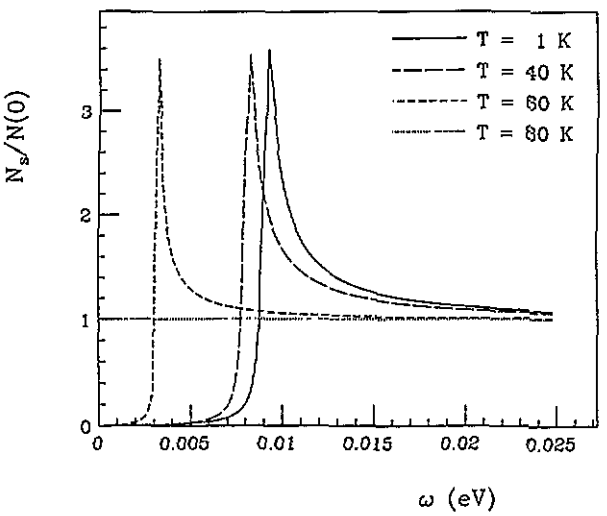

Figure 2. Reduced density of states of the superconducting state. $N(0)$ stands for the DOS of the non-superconducting state.

for larger values of the plasmon pole Ω, and in the limit we obtain a value of Ω for which the superconducting region is reduced to only one point. If one considers the temporal Fourier transformation of (7), the real part of the plasmon pole Ω gives the frequency of the resulting oscillating potential. In the cases with only one pole, $\pi/\mathrm{Re}\,\Omega$ will be the time interval in which the binding energy of the pair is different from zero, since during this time the potential is attractive. Therefore, the zone of the band parameters in which superconductivity is possible is more restricted (see figure 3) for increasing values of Ω and therefore for decreasing values of the periods in which the effective interaction is attractive.

The systematics for determining the transition temperature can be performed in a similar way to that given by McMillan [22], by considering in the integrand of (13) and (14) that

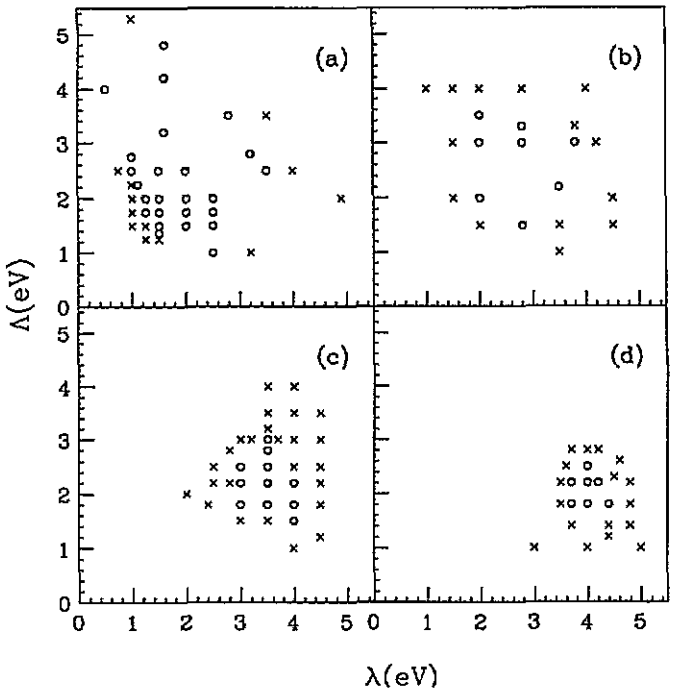

Figure 3. The zones of the drawing with circles are the regions of the band parameter space (λ and Λ are defined in the text) where superconductivity is possible. These regions are determined for different values of the oscillator frequency Ω (see (7)). (*a*) $\mathrm{Re}\,\Omega = 0.50$ eV, (*b*) $\mathrm{Re}\,\Omega = 0.85$ eV, (*c*) $\mathrm{Re}\,\Omega = 1.25$ eV, (*d*) $\mathrm{Re}\,\Omega = 1.5$ eV.

$W(\omega') \ll \omega' Z(\omega')$ for all ω' and thus, for $T \to T_c$,

$$W(\omega) = \int_{-\infty}^{\infty} A(\omega, \omega') W(\omega')\, \mathrm{d}\omega' \tag{16}$$

$$A(\omega, \omega') = K(\omega, \omega')\, \mathrm{Im} \int_{-\infty}^{\infty} \mathrm{d}x \frac{N(x)}{(\omega' + \mathrm{i}\delta)^2 Z(\omega')^2 - x^2} \tag{17}$$

$$S(\omega) = -\int_{-\infty}^{\infty} K(\omega, \omega')\, \mathrm{d}\omega'\, \mathrm{Im} \int_{-\infty}^{\infty} \frac{N(x)}{(\omega' + \mathrm{i}\delta) Z(\omega') - x}\, \mathrm{d}x. \tag{18}$$

Equation (16) is clearly an eigenvalue equation, where U^{-1} is the eigenvalue (we have to remark that $A(\omega, \omega')$ can be written as $A(\omega, \omega') = U\tilde{A}(\omega, \omega')$). $W(\omega)$ is in this equation the eigenvector, of infinite dimension. The value of $W(\omega)$ for $T \to T_c$ tends to zero for all ω. However, this equation will not be a null identity because if $W(\omega)$ is an eigenvector for a given eigenvalue U^{-1}, then any proportional vector $\alpha W(\omega)$ is also an eigenvector for the same U^{-1} value. We have therefore solved (16) self-consistently, fixing a T_c and determining the U value for which there is a convergent result of $\Delta(\omega)$. This calculation (see figure 4) allows us to give $U = U(T_c, \Omega, \lambda, \Lambda, n)$, and therefore $T_c = T_c(U, \Omega, \lambda, \Lambda, n)$.

In figure 4 we show the evolution of T_c versus U for different values of the width Λ of the Lorentzian DOS , using (16) and (17). The following points can be remarked: (i) for a given Λ, a minimum energy U is required to obtain superconductivity, (ii) for a given value of U, T_c increases for increasing values of Λ, and, therefore, for decreasing values of the DOS at E_F. This is physically meaningful, since superconductivity is a collective phenomenon, and the population of fermions near E_F determines the strength of the pair

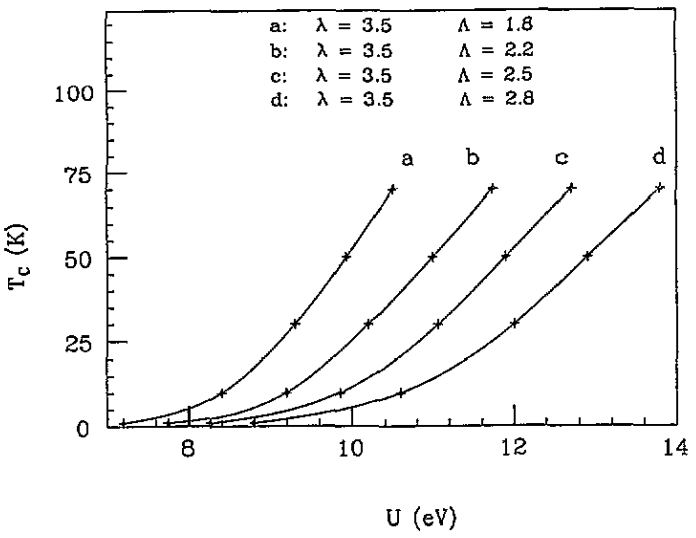

Figure 4. Evolution of T_c versus the energy U for different values of the Λ parameter.

potential for producing superconductivity. The results of figure 4 lead us to think that for U values between 9 and 12 eV, not far from estimated values for some strongly correlated systems, and reasonable band parameters for this type of material, T_c can reach about 90 K. However, it is necessary to remark that, in this theory, T_c is quite sensitive (see figures 3 and 4) to changes of the energy U and the other band parameters (Λ, λ, etc). In heavy-fermion systems, the DOS near E_F can be given by the Lorentzian curves with narrower widths and splitting between resonances at both sides of E_F, and therefore the characteristic transition temperatures are much lower.

We can conclude that our analysis indicates a way to solve the superconducting state within strongly correlated systems, and that high-T_c and heavy-fermion superconductivities can be considered as two different limits of the strongly correlated electron superconductivity, which could be explained from the strong-coupling equations, considering appropriate screenings of only one short-ranged repulsive interaction. This screening function should be determined by including in each case the corresponding characteristics of its electronic structure.

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