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Research Article

The link between *s* and *d* components of electron boson coupling constants in one band *d* wave Eliashberg theory for high T_c superconductors

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Abstract

The phenomenology of overdoped high T_c uperconductors can be described by a one band *d* wave Eliashberg theory where the mechanism of superconducting coupling is mediated by antiferromagnetic spin fluctuations and whose characteristic energy Ω_0 scales with T_c according to the empirical law $\Omega_0 = 5.8\ k_B T_c$. This model presents universal characteristics that are independent of the critical temperature such as the link between the *s* and *d* components of electron boson coupling constants and the invariance of the ratio $2\Delta/k_B T_c$. This situation arises from the particular structure of Eliashberg's equations which, despite being non-linear equations, present solutions with these simple properties.

Introduction

Eliashberg's theory [1] was born as a generalization of the BCS theory to explain some anomalies in the experimental data concerning lead. Subsequently, it was seen that the theory can be successfully applied to explain the experimental data of practically almost all superconducting materials [2,3], first of all low T_c phononic superconductors [4], then magnesium diboride [5,6], graphite intercalated compound CaC_6 [7], iron-based superconductors [8-12]. This theory can be applied to describe particular systems such as proximized systems [13] and field effect junctions [14-16]. For what concerns the high T_c superconductors [17-21], their properties strongly depend on their oxygen content. It is possible to identify three different regimes: under, optimal and overdoping. While the discussion is still open as regards the underdoping regime, it is almost certain that the fundamental mechanism in the optimal and over regime is due to antiferromagnetic spin fluctuations, and especially in the over regime, the experimental data can be described satisfactorily by one band *d* - wave Eliashbeg's theory [22,23]. Detailed studies are present in the literature on cuprates and precisely on tunneling spectra that can be reproduced by using the framework of *d* - wave Eliashbeg's theory [24-26]. In this paper, we provide an extensive investigation of the consequences of a different symmetry of coupling in the two components of self-energy: the renormalization function $Z(i\omega_n)$ (s-wave symmetry) and the gap function $\Delta(i\omega_n)$ (d-wave symmetry) and if some link exists between them. We focus here on physical quantities which can be evaluated in the imaginary axis formalism. Furthermore, it has been experimentally determined that, in cuprates, a link [27] exists between magnetic resonance energy Ω_0 and critical temperature. So we will study the properties of one band *d*-wave Eliashbeg's theory where a fundamental role will be played by the assumption that the representative energy Ω_0 of these systems is related to the critical temperature by

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a universal relationship [27] Ω_0 = 5.8 $k_B T_c$. This assumption represents a very strong constraint in correlating the values of the two-electron boson coupling constants λ_d and λ_s. For each value, λ_s we will look for the value λ_d which exactly reproduces the T_c superconductor and we will study which relation exists between the d and s components of the electron boson coupling constant. Finally, we will see that this model has the particular property that the relationship between the gap and the critical temperature ($\frac{2\Delta_d}{k_B T_c}$) is independent of the particular value of the critical temperature.

Model

The one-band d-wave Eliashberg equations [23,30-35] are two coupled equations: one for the gap $\Delta(i\omega_n,\phi)$ and one for the renormalization functions $Z(i\omega_n,\phi)$. These equations, in the imaginary axis representation (here ω_n denote the Matsubara frequencies), when the Migdal theorem holds [29], are:

$$\omega_n Z(\omega_n,\phi) = \omega_n + \pi T \sum_m \int_0^{2\pi} \frac{d\phi'}{2\pi} \Lambda(\omega_n,\omega_m,\phi,\phi') N_Z(\omega_m,\phi') \quad (1)$$

$$Z(\omega_n,\phi)\Delta(\omega_n,\phi) = \pi T \sum_m \int_0^{2\pi} \frac{d\phi'}{2\pi} [\Lambda(\omega_n,\omega_m,\phi,\phi') - \mu^*(\phi,\phi')] \times$$

$$\times \Theta(\omega_c - |\omega_m|) N_\Delta(\omega_m,\phi') \quad (2)$$

where $\Theta(\omega_c - \omega_m)$ is the Heaviside function, ω_c is cut-off energy and

$$\Lambda(\omega_n,\omega_m,\phi,\phi') = 2\int_0^{+\infty} \Omega d\Omega \alpha^2 F(\Omega,\phi,\phi') / [(\omega_n - \omega_m)^2 + \Omega^2] \quad (3)$$

$$N_Z(\omega_m,\phi) = \frac{\omega_m}{\sqrt{\omega_m^2 + \Delta(\omega_m,\phi)^2}} \quad (4)$$

$$N_\Delta(\omega_m,\phi) = \frac{\Delta(\omega_m,\phi)}{\sqrt{\omega_m^2 + \Delta(\omega_m,\phi)^2}} \quad (5)$$

We assume [2,23,30-35] that the electron boson spectral function $\alpha^2(\Omega)F(\Omega,\phi,\phi')$ and the Coulomb pseudopotential $\mu^*(\phi,\phi')$ at the lowest order contain separated s and d -wave contributions,

$$\alpha^2 F(\Omega,\phi,\phi') = \lambda_s \alpha^2 F_s(\Omega) + \lambda_d \alpha^2 F_d(\Omega) \sqrt{2} cos(2\phi) \sqrt{2} cos(2\phi') \quad (6)$$

$$\mu^*(\phi,\phi') = \mu_s^* + \mu_d^* \sqrt{2} cos(2\phi) \sqrt{2} cos(2\phi') \quad (7)$$

as well as the self-energy functions:

$$Z(\omega_n,\phi) = Z_s(\omega_n) + Z_d(\omega_n) cos(2\phi) \quad (8)$$

$$\Delta(\omega_n,\phi) = \Delta_s(\omega_n) + \Delta_d(\omega_n) cos(2\phi) \quad (9)$$

We put the factor $\sqrt{2}$ inside the definition $\Delta_d(\omega_n)$ because, experimentally, the peak of the density of the state is, usually, identified $\Delta_d(\omega_{n=0})$ while, as we will see, $Z_d(\omega_n)$ is always zero. The spectral functions $\alpha^2 F_{s,d}(\Omega)$ are normalized in the way that $2\int_0^{+\infty} \frac{\alpha^2 F_{s,d}(\Omega)}{\Omega} d\Omega = 1$ and of course, in this model the renormalization function is pure s-wave ($Z(\omega_n,\phi)$ = $Z_s((\omega_n))$ while the gap function is pure d-wave ($\Delta(\omega_n,\phi) = \Delta_d(\omega_n) cos(2\phi)$). We consider just solutions of the Eliashberg equations in pure d -waveform because this is the indication of the experimental data. This means that the s component of the gap function is zero and this situation happens because, usually [36], $\mu_s^* >> \mu_d^*$). In the more general case, in principle, the gap function has d and s components. The renormalization function $Z(\omega,\phi') = Z_s(\omega)$ has just the s component because the equation $Z_d(\omega_n)$ is a homogeneous integral equation with just the solution $Z_d(\omega_n)$ = 0 [37]. For simplicity, we also assume that $\alpha^2 F_s(\Omega) = \alpha^2 F_d(\Omega)$ the spectral functions are the difference between two Lorentzian, i.e. $\alpha^2 F_{s,d}(\Omega) = C[L(\Omega + \Omega_0, \Upsilon) - L(\Omega - \Omega_0, \Upsilon)]$ where $L(\Omega \pm \Omega_0, \Upsilon)) = [(\Omega \pm \Omega_0)^2 + (\Upsilon)^2]^{-1}$, C is the normalization constant necessary to obtain $2\int_0^{\infty} \frac{\alpha^2 F_{s,d}(\Omega)}{\Omega} d\Omega = 1$, $_0$ and γ are the peak energy and half-width, respectively. The half-width is $=\Omega_0/2$. This choice of the shape of the spectral function and the fact that $\alpha^2 F_s(\Omega) = \alpha^2 F_d(\Omega)$, is a good approximation of the true spectral function [38] connected with antiferromagnetic spin fluctuations. The same thing also happens in the case of iron pnictides [39]. In any case, even making different choices for γ the link between λ_d and λ_s) remains the same but changes (very little) the coefficients of the linear fit. The cut-off energy is $\omega_c = 1000$ meV and the maximum quasiparticle energy is ω_{max} = 1100 meV. In the first approximation, we put $\mu_d^* = 0$ (if the s component of the gap is zero the value of μ_s^* is irrelevant). Now we fix the critical temperature and for any value, λ_s we seek the value λ_d that exactly reproduces the initial fixed critical temperature. After, via Padè approximants [40], we calculate the low-temperature value (T = T_c/10 K) of the gap because, in presence of a strong coupling interaction, the value $\Delta_d(\omega_{n=0})$ obtained by solving the imaginary-axis Eliashberg equations can be very different from the value Δ_d obtained from the real-axis Eliashberg equations [31].

Results and discussions

We fix three different critical temperatures (70 K, 90 K and 110 K) and for any particular critical temperature, we choose different values λ_s and determine which value λ_d exactly reproduces the chosen critical temperature by numerical solution of Eliashberg equations. In Figure 1 we can see that

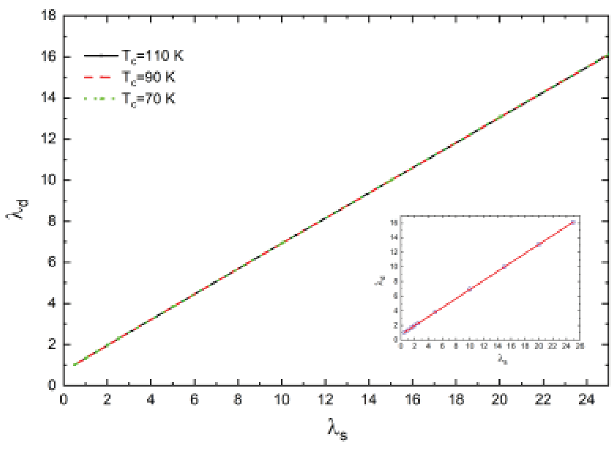

Figure 1: (Color online) λ_d versus λ_s for three different critical temperatures: T_c = 70 K (green point line), T_c = 90 K (red dash line) and T_c = 110 K (black solid line). In the inset the linear fit (solid line) of the T_c = 70 K (open dark blue circles) case is shown.

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the three curves λ_d *versus* λ_s are coincident. The inset of Figure 1 it is shown the linear fit of these results. We obtain a linear link between λ_d and λ_s

$$\lambda_d = 0.616\lambda_s + 0.732 \quad (10)$$

These results are general and do not depend on the particular shape of the electron-boson spectral function. If we change the shape of the electron-boson spectral function and we choose, for example, $\alpha^2F_{s,d}(\Omega) = 0.5\Omega_0\delta(\Omega-\Omega_0)$ we find that the linear link between λ_d and λ_s changes very little and becomes $\lambda_d = 0.575\lambda_s + 0.655$. Even the introduction of a Coulomb potential different from zero, as we have verified, does not involve a substantial modification of our results. In principle, it is possible to obtain this result (the linear link between λ_s and λ_d) in a more simple but less general way. In fact, a similar conclusion relative to the linear connection between λ_s and λ_d may also be derived from the analysis of the approximate MacMillan formula for T_c [41] generalized to d-wave case [42]:

$$k_BT_c = \Omega_0 exp(-\frac{1+\lambda_s}{2\lambda_d}) \quad (11)$$

The problem is that the MacMillan equation works just in a weak coupling regime. Now we solve, for each couple of λ_d and λ_s values, the Eliashberg equations at $T = T_c/10$ and after, via Pade we calculate the value of superconductive gap (the energy of the density of states peak). In Figure 2 the rates $\frac{2\Delta_d}{k_BT_c}$ are shown for three systems with different critical temperatures (70 K, 90 K and 110 K). The curves are exactly coincidental. We have also studied what happens when the ratio $\frac{\Omega_0}{k_BT_c}$ is equal to two as in the case of the heavy fermion [43] UPd_2Al_3 with T_c = 2 K which could represent an extreme situation. In this case, the link remains linear and becomes $\lambda_d = 0.880\lambda_s + 0.966$ as it is possible to see in the inset of Figure 2. Finally, in the case of extremely strong coupling ($\frac{\Omega_0}{k_BT_c} << 1$) it is possible to demonstrate in an analytical way, following the calculus of ref 26, when $\frac{\lambda_s}{2\lambda_d} > 1$, that $\lambda_d \approx \lambda_s$ i.e. the link remains linear.

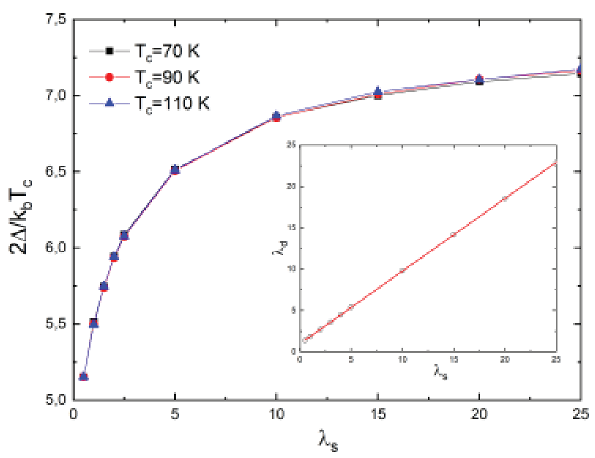

Figure 2: (Color online) $|\Delta_i|/k_BT_c$ for T_c= 70 K (green up filled triangles circles), T_c= 90 K (red filled circles) and T_c= 110 K (black filled squares) versus$|\lambda_s|$. The lines are guides for eyes. In the inset $|\lambda_d|$ versus $|_s|$ when T_c= 2 K and Ω_0= $2k_BT_c$ is shown (black open circles) with the linear fit (solid red line).

Conclusion

In this article, it has been shown that one band d-wave Eliashbeg's theory presents universal aspects as the linear link between λ_d and λ_s or the values $2\Delta_d/k_BT_c$ that are independent of the particular critical temperature. These universal aspects are related to the assumption that the typical bosonic energy is correlated to the critical temperature as shown by experimental data (Ω_0= 5.8 k_BT_c). We here proved that in a fully numerical solution of the Eliashberg equation, such linear links hold with great accuracy. A generalization and development of our results can be obtained by explicitly considering the momentum dependence of the self-energy without average on the Fermi surface as was done by Kamila A. Szewczyk, et al. [44]. Obviously, we would include in the calculations, unlike them, as we have done now, the link, observed experimentally, between the critical temperature and the representative energy of the bosonic spectrum.

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