Superconductivity in the presence of correlations

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A B S T R A C T

Following a two-pole approximation for strong correlations in the presence of superconductivity, we investigated the interplay between local repulsion and superconductivity, mainly on T_c, which is the superconducting critical temperature. In addition to correlations, we used a tight-binding band structure that considers hopping beyond the first nearest neighbors. Our approach is based on a doped Mott insulator, which has as its starting point the physics of strong correlations, which produces two Dirac delta functions for the spectral density. We conclude that correlations change the value of $T_{c,max}$ and the position of this maximum. Integration around the Fermi sea was carried out by including a cutoff frequency, ω_d. This work is mainly devoted to a superconductor with an order parameter of s-wave symmetry, which comes from a superconducting pairing potential, V, with $V \leq 0$. However, results for d-wave symmetry are also presented. Our results show that a mean-field treatment of correlations is not enough to completely understand these two mechanisms (superconductivity and correlations) where they act simultaneously.

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1. Introduction

The field of strongly correlated electron systems (*SCES*) has a very long history in condensed matter physics. Some of the most relevant works are the papers by Roth [1] and Edwards [2]. On the other hand, the field of superconductivity has developed separately since its discovery more than one hundred years ago, when Heike Kamerlingh Onnes discovered the lack of resistivity in Mercury in Holland. However, Bednorz and Müller discovered superconductivity in cuprates in 1986 [3] and the discovery of these new materials marked a new era for the field of condensed matter physics due to the combination of at least three factors: first, high values of the superconducting critical temperature, T_c; second, the presence of correlations ranging from intermediate to strongly correlated regimes; third, anomalous properties below a certain energy scale, named $k_B\,T^*(x)$, where k_B is the Boltzmann constant, $x = |1 - n_T|$ is the doping of the copper oxide plane with electrons or holes [3] and n_T is the number of carriers. In other words, in the interplay of superconductivity and electron correlations, there can be two possible scenarios: in the first one, the correlations survive up to the superconducting dome. In the second scenario the correlations survive inside the superconductor regime. For a discussion of these scenarios, see Tallon and Loram [4]. Varma [5] has studied the mechanisms and the transition temperatures for superconductivity induced by electronic fluctuations. Evidence of strong correlations inside the superconducting region led us to adopt the second scenario.

Let us say, before getting into the main issue of this paper, that previous approaches have tackled correlations, such as [6–8], among others. In particular, Ref. [7] uses the Hubbard-I approximation [9]. In Ref. [10], Díaz et al. studied the presence of correlations for an s-wave order parameter symmetry at $T = 0$. W. Nolting [11] uses the moment approach for treating only the Hubbard hamiltonian, namely, the term with $U > 0$ (U is the Coulomb potential).

Due to the possibility of studying physical systems where correlations are at the intermediate to strong coupling limit, without reaching the atomic regime, we have employed the method of Roth [1] and her followers [2,12,13]. As the cuprate superconductors have a rich phase diagram, with different energy scales, we have used two parameters to study them, U and V, for correlation and pairing, respectively (see also, Ref. [14]).

The cuprate superconductors [3], the materials we had in mind in the development of this study, show a rich phase diagram, i.e., T vs x (doping), which lacks a clear understanding and explanation even after twenty-nine years of investigation. Therefore, we chose to adopt a phenomenological model that includes an effective parameter for electronic correlations, $U > 0$, and another parameter that accounts for superconductivity, denoted as $V < 0$. Our attractive potential, $V < 0$, can be justified by the three orbital model [15,16] of Emery. Also, this attractive interaction may be attributed

to a bosonic mechanism with phonon-like or spin-like exchange. See Ref. [17], where the exchange energy giving rise to superconductivity could be attributed to different mechanisms.

In what follows, U is the highest energy scale of our problem, for which a mean-field treatment is not valid. So, we use the treatment of Roth [1] and followers [2,12,13]. For the case of $V < 0$ we employ a mean-field treatment. Roth's method has been proposed to improve the Hubbard-I approximation [9]. In the Hubbard approximation, the third moments of the Green's functions have not been obtained. The procedure proposed by Roth gives rise to an energy shift in the self-energy leading to an adequate treatment of third order moments. The spin dependence of the band shift, due to the presence of the intersite correlation function $\langle \vec{S}_j \cdot \vec{S}_i \rangle$, allows for magnetic (ferromagnetic and antiferromagnetic) solutions in the one-band Hubbard model, while this feature is not present in the Hubbard-I solution. Roth's method has been used in reference [2] to study the normal and superconducting properties of the Hubbard model. The results were compared with those obtained by Monte Carlo calculations showing that the quasi-particle bands and the spectral weights are in good agreement.

The phase diagram of the cuprate superconductors (T vs x), where correlations are important, presents an energy scale known as the pseudogap temperature (T_p)/energy (E_p), given by $E_p = k_B T_p$ in the doping regime of $0 < x \lesssim 0.20$. Even though we consider that in our model the basic parameters are U and V, we also indicate the importance of the chosen band structure, which is obtained from spectroscopic measurements. The effect of the band structure on T_c is not included here.

With these two parameters at hand, plus the tight-binding structure of Norman et al. [18], we start our study of superconductivity (mean-field approach) in the presence of strong local repulsion (beyond mean-field treatment). U is entirely included in the two-pole ansatz chosen. To include it in a mean-field treatment of superconductivity will produce double-counting, which must be avoided. With this in mind, the two mechanisms satisfy the six first moments in the language of Nolting [11], four for the correlations and two for superconductivity. The electronic band is split in two: the lower Hubbard band and the upper Hubbard band.

We have two mechanisms at work, the pairing one and the repulsive interaction. Even having strong electronic correlations, the fermionic nature of the system remains as is recognized by Norman and Proust [19] who affirm that the origin of the high T_c remains an enigma. But it is possible to discuss the "*fermionlogy*" of the cuprates thanks to the discovery of quantum oscillations, which give valuable information about the Fermi surface and therefore the physical properties of a metal. Even in the presence of interactions, the concept of a Fermi surface remains robust. Over much of the phase diagram, the normal state exhibits an energy gap [20].

In 2007 a breakthrough occurred with the unambiguous observation of quantum oscillations in underdoped (*UD*) $YBa_2Cu_3O_{6.5}$. This effect is a direct consequence of quantization of closed cyclotron orbits, establishing the existence of a well-defined Fermi surface in the ground-state of the *UD* cuprates.

On the other hand, Atkinson, Kamp and Bulut [21] have studied the effect of a charge order in the pseudogap phase of the cuprate superconductors. As the Cu–O planes have three orbitals per unit cell, they consider that the large local Coulomb interaction in the $Cu - d_{x^2-y^2}$ orbitals generates local moments with short-range antiferromagnetic correlations. These antiferromagnetic interactions lead to a *PG*-like reconstruction of the Fermi surface. We do not consider the role of the pseudogap in our present calculations.

The present work aimed to employ an adequate technique [1, 2] to observe the effect of strong correlations on superconductivity, i.e., $T_c = T_c(U)$. The pseudogap issue should be addressed in a forthcoming work.

In Section 2 we present Roth's approximation, which is valid in the intermediate to strong coupling regime ($\infty > U/t \geq 1$), where U is the local electron repulsion and t is the hopping integral between nearest neighbors (*n.n.*). In our case, we have used the band structure (tight binding) of Norman et al. [18]. After solving the self-consistent equations of Section 2 by numerical means, we present the numerical results in Section 3. Section 4 is devoted to conclusions. We leave for the Appendix A the details of the different terms present in our self-consistent equations (Section 2), which might deviate from the main line of thought around the interpretation given in Section 3.

2. The general formulation

As we have said in the Introduction, we will consider a phenomenological model in which we have two free parameters, $U > 0$ which is of Coulomb-type. According to our considerations we do not touch the atomic limit. The high values of U/t produce a band-narrowing which can be visualized as the starting point of Micnas, Ranninger and Robaskiewicz [22] and other [23,24]. On top of this narrow-band structure we have a second phenomenological parameter, $V < 0$, with $1 \leq |V|/t \ll U/t$, which gives origin to superconductivity.

Thus, we exactly solve the diagonal one-particle Green function,

$$G_\sigma(\vec{k}, \omega) = \frac{Z_{1,\sigma}(\vec{k})}{\omega - E_{1,\sigma}(\vec{k})} + \frac{Z_{2,\sigma}(\vec{k})}{\omega - E_{2,\sigma}(\vec{k})} \ , \tag{1}$$

which produces the following spectral function, $A_\sigma(\vec{k}, \omega)$ given by

$$A_\sigma(\vec{k}, \omega) = Z_{1,\sigma}(\vec{k})\delta\left(\omega - E_{1,\sigma}(\vec{k})\right) + Z_{2,\sigma}(\vec{k})\delta\left(\omega - E_{2,\sigma}(\vec{k})\right) \ , \tag{2}$$

where $\delta(x)$ is the Dirac delta function of argument-x. $Z_{i,\sigma}(\vec{k})$ are the spectral weights for each Hubbard band, $i = 1, 2$ and spin, σ.

After substituting the one-particle Green function in the self-consistent equations for the particle number, n_T, and the superconducting order parameter, $\Delta(\vec{k})$, at the superconducting critical temperature $T = T_c$, we come out with the following self-consistent equations:

$$n_T = 2 \int_0^\pi \frac{d^2\vec{k}}{\pi^2} \left[1 - Z_{1,\sigma}(\vec{k})A_\sigma(\vec{k}) - Z_{2,\sigma}(\vec{k})B_\sigma(\vec{k}) \right] \tag{3}$$

and

$$\frac{1}{V} = \int_0^\pi \frac{d^2\vec{k}}{\pi^2} \Bigg\{ 1 - Z_{1,\sigma}^2(\vec{k})A_\sigma(\vec{k}) - Z_{2,\sigma}^2(\vec{k})B_\sigma(\vec{k})$$
$$+ \frac{2Z_{1,\sigma}(\vec{k})Z_{2,\sigma}(\vec{k})}{E_{1,\sigma}(\vec{k}) + E_{2,\sigma}(\vec{k})} \left[A_\sigma(\vec{k}) + B_\sigma(\vec{k}) \right] \Bigg\} \varphi^2(\vec{k})\psi(\vec{k}) \tag{4}$$

with,

$$A_\sigma(\vec{k}) = \tanh\left(\frac{E_{1,\sigma}(\vec{k})}{2k_B T_c} \right) \tag{5}$$

and

$$B_\sigma(\vec{k}) = \tanh\left(\frac{E_{2,\sigma}(\vec{k})}{2k_B T_c} \right) \tag{6}$$

where $Z_{i,\sigma}$ and $E_{i,\sigma}$ are defined in Appendix A.

Also,

$$\varphi(\vec{k}) = \begin{cases} 1 & \rightarrow s\text{-wave} \\ \cos(k_x) - \cos(k_y) & \rightarrow d\text{-wave} \end{cases}$$