s–wave superconductivity in the presence of local Coulomb correlations

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We derive the superconducting mean–field equations for an attractive interaction, $V$, in the s–wave channel when local Coulomb interactions are taken into account for any value of $U$. Our results show that the Coulomb repulsion is detrimental to the critical temperature, $T_c$, and the order parameter, $\Delta(T)$, for values of $U \geq |V|$. Furthermore, our results depend on band filling in a sensible way. In the presence of local correlations, $2\Delta(0)/T_c$ differs from the BCS ratio, since Coulomb interactions affect much more the superconducting critical temperature, $T_c$, than the superconducting order parameter, $\Delta(T)$. We conclude that the presence of Coulomb interactions play an additional role in the analysis of experimental data, specially in narrow band systems.

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The discovery of high–$T_c$ superconductors (HTSC) [1] has given a huge impetus to the theory of correlation effects [2] due to the fact that there is the belief [3] that the normal properties of these materials could be explained in the framework of the Hubbard model [4,5], since electron correlations are strong, i.e., the on-site electron-electron repulsions $U$ are much larger than the energies associated to the hybridization of atomic orbitals belonging to different atoms. Two dimensional (2–D) Mott–Hubbard insulators exhibit unconventional electronic, optical, and magnetic behavior when doped with mobile charge carriers. However, subsequent analytical and numerical work lead to the conclusion that the possibility of superconductivity order out of purely repulsive interactions is not conclusive. So, the mechanism of the HTSC is still elusive after almost thirteen years of intense research and extensions to the pure Hubbard model have been used [6]. See also Ref. [7]. Due to this lack of consensus an additional phenomenological interaction has to be included to go into the superconducting phase. Because of that, following Ref. [7], we postulate a Hamiltonian which is composed of two terms, the Hubbard contribution, which we call interaction has to be included to go into the superconducting phase. Because of that, following Ref. [7], we postulate a Hamiltonian which is composed of two terms, the Hubbard contribution, which we call interaction has to be included to go into the superconducting phase.

Due to the fact that there has been a large amount of studies in the normal state of the HTSC, we consider that the normal state Green function is known and we tackle the superconducting state by means of a mean–field treatment. For the normal state Green function, for all values of $U$, we choose an academic Hubbard–III like approximation [10] which gives a metal for small values of $U$ (no gap in the density of states) and becomes an insulator for large values of $U$ (there is a gap for $U \geq W$, where $W$ is the band width). Our studies differ from the ones recently published in the literature where mean field analysis has been performed for both $U$ and $V$ [11,12]. We then find the diagonal and off–diagonal superconducting one–particle Green functions, $G(\vec{k}, i\omega_n)$ and $F(\vec{k}, i\omega_n)$, respectively. Using these two Green functions, we derive the self–consistent equations for the density and the gap equation, respectively. These equations are self–consistent and we have solved them numerically.

In the superconducting phase, we will follow the BCS treatment supposing that the presence of correlations leave this formalism untouched [1]. Our dynamical equations become

$$G_U^{-1}(\vec{k}, i\omega_n)G(\vec{k}, i\omega_n) + \Delta(T)F^+(\vec{k}, i\omega_n) = 1,$$

$$G_U^{-1}(\vec{k}, i\omega_n)F^+(\vec{k}, i\omega_n) - \Delta(T)G(\vec{k}, i\omega_n) = 0,$$

with $G_U(\vec{k}, i\omega_n)$ being the normal state correlated one–particle Green function [11,13]

$$G_U(\vec{k}, i\omega_n) \equiv \frac{1 - \rho}{i\omega_n + \mu - \epsilon(\vec{k})} + \frac{\rho}{i\omega_n + \mu - \epsilon(\vec{k}) - U},$$

$\epsilon(\vec{k})$ being the free band structure, $\rho$ is the particle density/spin and $\omega$ is the fermionic (odd) Matsubara frequency. According to our interpretation, the Hamiltonian is split in two pieces.
\[ H = H_U + H_V \]  

where \( H_U = H_o \) is our unperturbed Hamiltonian for which we know the solution in the normal state. This is the reason of having chosen the normal Green function as in Eq. (3). Of course, we do not know the exact solution of the Hubbard model even in \( d \equiv \infty \) due to the local character of the Coulomb interaction. However, if we have a normal Green function which interpolates between the weak and the strong coupling regime, then we can say that we have a pretty good solution to the the Hubbard part. According to this view what we are studying is the effect of Coulomb interactions, \( U \), on superconductivity. We mention that there are other types of approximations for \( G_U(\vec{k}, i\omega_n) \) as it has been done in Ref. [11], i.e., Hartree–Fock (HF), second order perturbation theory (SOP'T) and the alloy analogy approximation (AAA) [14]. The way to view Eq. (2) in terms of Feynman diagrams is the following: our internal lines are due to correlated Green functions, due to \( G_U(\vec{k}, i\omega_n) \), and the vertex or interaction is due to the Cooper interaction, \( V \).

Solving Eqs. (1), we get

\[
G(\vec{k}, i\omega_n) = \frac{G^{-1}_U(\vec{k}, i\omega_n)}{G^{-1}_U(\vec{k}, -i\omega_n) + |\Delta(T)|^2},
\]

\[
F^\dagger(\vec{k}, i\omega_n) = \frac{\Delta^*(T)}{G^{-1}_U(\vec{k}, i\omega_n)G^{-1}_U(\vec{k}, -i\omega_n) + |\Delta(T)|^2}.
\]  

Before showing our working equations, it is instructive to elaborate a little further our superconducting Green functions, expressing them in terms of their poles and their residues. The result of this is the following

\[
G(\vec{k}, i\omega_n) = \frac{\alpha_1}{i\omega_n - Y_1^n} + \frac{\alpha_2}{i\omega_n + Y_1^n} + \frac{\alpha_3}{i\omega_n - Y_2^n} + \frac{\alpha_4}{i\omega_n + Y_2^n};
\]

\[
F^\dagger(\vec{k}, i\omega_n) = -\Delta^*(T) \left[ \frac{\beta_1}{i\omega_n - Y_1^n} - \frac{\beta_1}{i\omega_n + Y_1^n} + \frac{\beta_2}{i\omega_n - Y_2^n} - \frac{\beta_2}{i\omega_n + Y_2^n} \right].
\]

The notation is explained in Eqs. (6). The reason of having four poles is because the denominator of \( G(\vec{k}, i\omega_n) \) and \( F^\dagger(\vec{k}, i\omega_n) \) is a polinomial of order four.

Substituting \( G_U(\vec{k}, i\omega_n) \) from Eq. (2) we find the mean-field equations for \( \Delta(T) \) and \( \rho \), respectively, as

\[
\frac{1}{V} = -\frac{1}{2D} \int_{-D}^{+D} \left[ \beta_1(x) \tanh\left( \frac{Y_1(x)}{2T} \right) + \beta_2(x) \tanh\left( \frac{Y_2(x)}{2T} \right) \right] dx,
\]

\[
\rho = \frac{1}{2D} \int_{-D}^{+D} \left[ \alpha_1(x)f(Y_1(x)) + \alpha_2(x)f(-Y_1(x)) + \alpha_3(x)f(Y_2(x)) + \alpha_4(x)f(-Y_2(x)) \right] dx,
\]

where we have chosen a flat free density of states, i.e., \( N_L(\epsilon) = 1/2D \) for \( -D \leq \epsilon \leq +D \) and zero otherwise. In the end we have chosen \( 2D = 1 \). The notation in Eq. (6) is as follows

\[
f(x) = \frac{1}{\exp(x/T) + 1}; \quad \beta_1 = \frac{Y_1^2 - \tilde{x}_1^2}{2Y_1(Y_1^2 - \tilde{x}_1^2)}; \quad \beta_2 = \frac{Y_2^2 - \tilde{x}_1^2}{2Y_2(Y_2^2 - \tilde{x}_1^2)};
\]

\[
x_1 = \mu; \quad \tilde{x}_1 = x_1 + U; \quad \bar{x}_1 = x_1 + (1 - \mu)U;
\]

\[
\alpha_1(x_1, \tilde{x}_1, \bar{x}_1) = \frac{(Y_1 + x_1)(Y_1 + \bar{x}_1)(Y_1 - \tilde{x}_1)}{2Y_1(Y_1^2 - \tilde{x}_1^2)}; \quad \alpha_2 = \alpha_1(-x_1, -\tilde{x}_1, -\bar{x}_1);
\]

\[
\alpha_3(x_1, \tilde{x}_1, \bar{x}_1) = \frac{(Y_2 + x_1)(Y_2 + \bar{x}_1)(Y_2 - \tilde{x}_1)}{2Y_2(Y_2^2 - \tilde{x}_1^2)}; \quad \alpha_4 = \alpha_3(-x_1, -\tilde{x}_1, -\bar{x}_1);
\]

\[
Y_{1,2}^2 = \frac{1}{2} \left[ \tilde{x}_1^2 + \bar{x}_1^2 + |\Delta|^2 \pm \left( \tilde{x}_1^2 + \bar{x}_1^2 + |\Delta|^2 \right)^{1/2} \right].
\]

From our previous expressions we can verify that

\[
\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 = 1; \quad Y_1(\alpha_1 - \alpha_2) + Y_2(\alpha_3 - \alpha_4) = \epsilon(\tilde{k}) + \rho U.
\]

Eqs. (5) are nothing that the first two sum rules or moments of the diagonal spectral function, \( A(\vec{k}, \omega) = -1/\pi \lim_{\delta \to 0^+} \text{Im} \left[ G(\vec{k}, \omega + i\delta) \right] \). We see that the presence of Coulomb correlations yields \( \alpha_1 \neq \alpha_2 \) and \( \alpha_3 \neq \alpha_4 \).
Analyzing our gap equation we see that the BCS energy symmetry is kept, i.e., we have the following one–particle energy excitation solutions, ±Y₁, and ±Y₂ (the last line of Eq. (3)). By the same token, the off–diagonal spectral function, \( B(\vec{k}, \omega) = -1/\pi \lim_{\delta \to +0} \text{Im} \left[ F(\vec{k}, \omega + i\delta) \right] \) complies with the first two off–diagonal sum rules. These considerations are a check that we are working in a mean field scheme for the superconducting one–particle Green functions, as it should be. To go beyond the mean–field solution, we need to include pairing fluctuations as it has been done by Micnas et al of Ref. [13]. Also, pairing fluctuations have been studied by Schmid [16] and others [17,18].

In Fig. 1 we present \( T_c \) vs \( \mu \) for various values of \( \mu \), i.e., \( \mu = 0.25; 0.50; 0.75 \) and 1.00, for several values of \( V \), i.e., \( V = -0.50; -1.00; -1.50 \) and -2.00. We immediately conclude that \( T_c \) goes to zero for high values of \( \mu \). Also, we observe that, for chosen values of \( V \), there is a maximum value of \( \mu \approx 1.4 \) beyond which there is no superconductivity. We gain these results by taking \( \Delta(T) = 0 \) in Eqs. (3). Fig. 1 is our guiding line for solving Eqs. (3) below \( T_c \), i.e., we will use the parameters of Fig. 1 and solve \( \Delta(T) \neq 0 \) for \( T \leq T_c \).

For example, in Fig. 2 we plot \( \Delta(T)/U \) vs \( T/T_c \) for various values of \( U \) and \( \mu = 0.50 \). For all our curves, \( \Delta(T)/U \) goes down when \( U \) increases. This can be explained because \( \Delta(T) \) is a parameter which is conceptually defined thru \( |V| \), i.e., it depends little on \( U \). When we normalize \( \Delta(T) \) with \( U \), we are decreasing this ratio drastically. For high values of \( U \), \( \Delta(T)/U \) goes to zero. We see that for \( U = 1.0 \) the value of the normalized gap, i.e., \( \Delta(T)/U \), is almost zero. However, if the value of \( |V| \) is comparable to \( U \) then we can have a sizeable value of the normalized ratio. So, there are two competing parameters in the theory, \( U \) and \( V \), which are controlling the value of the order parameter.

In Fig. 3 we present \( \Delta(T)/\Delta_{max} \) vs \( T/T_c \), where \( \Delta_{max} \equiv \Delta(0) \). \( T_c \) is the value given in Fig. 1. We see that the outmost curve is the one with \( U = 0 \) (pure BCS case) and the inmost curve is the one with the highest value of \( U \). Thus, for high values of \( U \), \( \Delta(T)/\Delta_{max} \) decreases in the intermediate region, i.e., for \( 0 < T < T_c \). So, superconductivity is basically diminished for high values of \( U \), a result which had been reached in previous works [11,12]. In particular, for \( \mu = 0.50 \), and \( U = -1.00 \) there is a great deviation with respect to the pure BCS case (\( \mu = 0 \)). This fact should be detected experimentally. Fig. 3 is particularly illuminating because depending on band filling (or \( \mu \) and certain values of \( U \) we can deviate from the pure BCS result. Of course, there is an additional difference with respect to the \( U = 0 \) case: we have two different excitation energies, namely \( Y_1 \) and \( Y_2 \) (Eq. (3)).

In addition, we have evaluated \( 2\Delta(0)/T_c \). In pure BCS, it is approximately equal to \( 3.5 \). For \( \mu = 0.25 \), \( V = -0.50 \), \( U = 0.25 \) (\( \rho \approx 0.6 \)), we get that this ratio is \( \approx 4.37 \). Also, for \( \mu = 0.50 \), \( V = -0.50 \), \( U = 0.75 \) (\( \rho \approx 0.57 \) this ratio is \( \approx 6.585 \). As we have mentioned before, \( \Delta(T) \) is a quantity which is defined mainly thru the pairing interaction, \( V \). So, it does not change too much with \( U \). On the contrary, \( U \) has a bigger effect on \( T_c \) reducing it. This argument may explain the reasons why the \( 2\Delta(0)/T_c \) can be very different from the pure BCS ratio. In other words, the presence of Coulomb interactions plays a fundamental role in changing the universal ratio. We also see that the band filling, in presence of Coulomb interactions, plays a sensible role too. These results may have some relationship with one of the characteristic features of superconductivity in the cuprate superconductors: the strong dependence of \( T_c \) and \( \Delta(T) \) on doping concentration, \( x \), away from half filling (\( n = 2\rho = 1 - x \) [19]). But, above all, what we are led to is to see that the ratio \( 2\Delta(0)/T_c \) is no longer universal and changes with doping, for example. This has very important experimental consequences since we do not need to consider non–BCS theories to explain these big ratios. However, we can say that in our approach the Coulomb interaction plays an equivalent role of the \( \text{Non} – \text{Fermi Liquid} \) parameter \( \alpha \) of Refs. [15], namely, they decrease the value of \( T_c \).

In short, we have solved the gap and density equations inside the superconducting phase for \( s \)-wave symmetry order parameter taking into account local Coulomb repulsion of any strength. Speaking a little bit about numerics, we say that we have paid due care to the cases \( Y_1 = Y_2 \) and \( Y_2 = 0 \). Also, for small values of \( \Delta(T) \) convergence depends on the initial conditions. The presence of electron correlations is detrimental to superconductivity. When we say that \( U \) conspire against superconductivity, one is saying that it diminishes both \( T_c \) and \( \Delta(T) \). For the first part of this statement, we show Fig. 1, which we use as our reference. The second part of the statement is shown in Figs. 2 and 3. At this point we call the attention of the reader to the point that our calculations were done at fixed \( \mu \). When \( U \) is taken into account, \( \mu \) (or band filling) starts to play a decisive role. In particular, we have found \( 2\Delta(0)/T_c > 3.5 \) which has also been found in experimental measurements. We could tried another type of normal state one–particle Green functions, instead of the one of Eq. (3). We leave this task for the future. We have said that our choice for the normal one–particle Green function, \( G_N(\vec{k}, i\omega_n) \), is an academic one because the weights of the spectral function, \( A(\vec{k}, \omega) \), are \( 1 - \rho \) and \( \rho \), respectively. In other words, we do not have \( \vec{k} \)-dependence which is a vital ingredient to explain angle–resolved photoemission (ARPES) data [20] of HTSC. However, our aim was to study the effect of \( U \) on the superconductivity parameters \( T_c \) and \( \Delta(T) \). Then, other better approximations can be used as it has been done in Ref. [11]. Furthermore, one could use the two–pole Ansatz of Nolting [15] which may give a normal state metal–insulator transition if the band narrowing band factor, \( B_N(\vec{k}) \), is properly treated. However, the basis physics will remain the same. Another point which has not been considered here is the effect of the lattice structure [21].

3
This paper has dealt with the isotope coefficient is a problem worthwhile to explore as well as the jump on the specific heat at $T = T_c$ [23]. This paper has dealt with the $s$-wave order symmetry only. However, complex symmetry [25] order parameter [25] do not represent numerical difficulty. See also, Ref. [26].

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[1] J. Bednorz and K.A. Müller, Z. Phys. B 64, 189 (1986)
[2] P. Fazekas, Lecture Notes on Electron Correlation and Magnetism. World Scientific (1999). Chapter 1
[3] P.W. Anderson, Science 235, 1196 (1987): Frontiers and Borderlines in Many Particle Physics. North Holland, Amsterdam (1988).
[4] J. Hubbard, Proc. R. Soc. London A 276, 238 (1963).
[5] J. Hubbard, Proc. R. Soc. London A 281, 401 (1964).
[6] Peter Fulde, Electron Correlations in Molecules and Solids. Springer-Verlag (1993). 2nd Edition.
[7] F. F. Assaad and I. Imada, Phys. Rev. B 58, 1845 (1998)
[8] L. Arrachea and A. A. Aligia, Phys. Rev. B 59, 1333 (1999). These authors use an additional correlated hopping term and $n.n.$ hopping $t'$. Their starting Hamiltonian is different from the previous reference [13]
[9] P. A. Anderson, The Theory of Superconductivity in the High-T$_c$ Cuprates. Princeton University Press (1997)
[10] M.A. Ikeda, U. Larsen and R. D. Mattuck, Phys. Lett. A 39, 55 (1972); R. Kishore and E. Granato, J. Phys.: Condens. Matter 2, L5633 (1990)
[11] T. Domaniński and K.I. Wysokiński, Phys. Rev. B 59, 173 (1999)
[12] J. J. Rodríguez–Núñez and A. A. Schmidt, unpublished (1999)
[13] J. J. Rodríguez–Núñez, M. S. Figueira, E. V. Anda and C. I. Ventura, Unpublished (1999)
[14] The AAA approximation has been recently revised and improved by M. Pottoff, T. Herrmann and W. Nolting, Eur. Phys. J. B 4, 485 (1998). This improvement allows to recuperate Fermi liquid behavior for small values of $U$ in the normal phase and the two well defined branches in the spectral density for large values of $U$. So, this approximation agrees with our choice made in Eq. (3), since the normal state Green function, $G_N(\vec{k}, \omega_n)$, forms part of our Hamiltonian $H_n$. We can treat $H_V$ in mean field
[15] W. Nolting, Z. Physik 255, 25 (1972); W. Nolting, Grundkurs: Theoretische Physik. 7 Viel-Teilchen-Theorie. Verlag Zimmermann-Neufang (Ulm-1992); R. Micnas, M. H. Pedersen, S. Scharfroth, T. Schneider, J. J. Rodríguez–Núñez and H. Beck, Phys. Rev. B 52, 16223 (1995); T. Schneider, M. H. Pedersen and J. J. Rodríguez–Núñez, Z. Phys. B 100, 263 (1996)
[16] A. Schmid, Z. Physik 321, 324 (1970)
[17] M. Crișan, C. P. Moca and I. Tîfrea, cond-mat/9809152
[18] L. Yin and S. Chakravarty, Int. J. Mod. Phys. B 10, 805 (1996); I. Tîfrea, I. Grosu and M. Crișan, Physica B 259–261, 464 (1999); V. N. Muthukumar, D. Sa and M. Sardar, Phys. Rev. B 52, 9647 (1995); I. Grosu, I. Tîfrea and M. Crișan, J. Supercond. 11, 339 (1998)
[19] S. Doniach and E. H. Sondheimer, Green's Functions for Solid State Physics. Imperial College Press (1998). Chapter 12
[20] Z. X. Shen et al, Phys. Rev. Lett. 70, 1553 (1993); ibid., Science 267, 343 (1993); ibid., Phys. Rev. Lett. 76, 4841 (1996)
[21] R. Kirchofer, R. Frésard, H. Beck and J.J. Rodríguez–Núñez, Physica B 259–261, 775 (1999); R. Kirchofer, Diplôme. Université de Neuchâtel (1997). Unpublished. In his Diplôme, Kirchofer started to study superconductivity in the presence of $U$ using the normal state Green approximation of Nolting [15]
[22] M. C. Refolio, J. M. López Sancho, J. Rubio and M. P. López Sancho, Phys. Rev. B 59, 5384 (1999)
[23] R. Kishore, Physica C 23, 367 (1995); R. Kishore and S. Lamba, Europhys. J. B 8, 161 (1999)
[24] P. Pureur. Private communication. He has however warned that the measurement of this quantity in a strongly correlated system (or HTSC) is a difficult task because the electronic specific heat, $C_V^e$, represents only two percent of the total specific heat, $C_V$.
[25] H. Ghost, Europhys. Lett. 43, 707 (1998) and private communication.
[26] K. Maki and M.T. Béal–Monod, Phys. Rev. B 55, 11730 (1997)

Figure Captions

Figure 1. $T_c$ vs $U$, for different values of $V$, i.e., $V = -0.50; -1.00; -1.50$ and $-2.00$. (a) $\mu = 0.25$; (b) $\mu = 0.50$; (c) $\mu = 0.75$; and (d) $\mu = 1.00$.

Figure 2. $\Delta(T)/U$ vs $T/T_c$ for several values of $U$ and four values of $V$, i.e., (a) $V = -0.50$; (b) $V = -1.00$; (c) $V = -1.50$; (d) $V = -2.00$. Here we have fixed the chemical potential to $\mu = 0.50$.

Figure 3. $\Delta(T)/\Delta_{max}$ vs $T/T_c$ for several values of $U$ and four values of $V$, i.e., (a) $V = -0.50$; (b) $V = -1.00$; (c) $V = -1.50$; (d) $V = -2.00$. We have again fixed the chemical potential to $\mu = 0.25$. 
