We constructed the one-particle spectral functions (diagonal and off-diagonal) which reproduce BCS for weak coupling and which take into account the effect of correlations on superconductivity in the attractive Hubbard model. The diagonal spectral function is composed of three peaks and the off-diagonal one is composed of two peaks. This ansatz satisfies the sum rules for the first six moments. Our solutions are valid for intermediate coupling, i.e., for $U/t \approx -4.0$. Our set of analytical equations for the unknown variables is self-consistent and has been solved numerically in lowest order of the order parameter. As a result, we obtain that the presence of the third band, or upper Hubbard band, strongly renormalizes the two lower bands, making that the energy gap be $k$-dependent while the order parameter is pure $s$-wave. This shows that the order parameter and the gap are two different quantities.

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The study of correlations has been renewed again by the discovery of high $T_c$ superconducting oxide materials (HTSC), since these materials exhibit a short coherence length, $\xi$, and a very large penetration depth, $\lambda$, thus behaving like extreme type-II superconductors, i.e. $\kappa \equiv \lambda/\xi \gg 1$. We will use the on-site attractive Hubbard Hamiltonian put forward by Micnas et al \cite{Micnas} as a phenomenological model for describing the HTSC. Previous authors have used this model to study the bismuthate superconductors. \cite{Bismuth}\ The importance of the Hubbard model has been recognized by Denteneer et al \cite{Denteneer} who say that if the phase diagram of the Hubbard model were fully understood, it might form the basis of understanding correlated electrons as much as the Ising model did for understanding critical phenomena. Schneider et al \cite{Schneider} have applied this model to explain universal properties of several families of these compounds, like the relation between transition temperature, magnetic penetration depth and gap, at zero temperature. It is likely that understanding this will provide insight into the effect of correlations on measurable quantities as shown by Singer et al \cite{Singer}.

We will use the exact relations of Nolting \cite{Nolting} for the one-particle diagonal spectral function together with the exact relations for the one-particle off-diagonal spectral function, i.e., the anomalous Green’s function, to study systems with broken symmetry. \cite{Nolting}\ We will start from the dynamical equations constructing one-particle Green’s functions which reduce to the BCS solution in the case of weak coupling. Our solutions, even in the case of BCS, give in a natural way the Hartree shift to the chemical potential.

The Hamiltonian we study is the following

$$H = -t \sum_{<i,j>\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_{i\sigma} ,$$

where $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) are creation (annihilation) electron operators with spin $\sigma$, $n_{i\sigma} \equiv c^\dagger_{i\sigma} c_{i\sigma}$, $t$ is a hopping matrix element between the nearest sites $i$ and $j$, and $U$ is the onsite interaction. $\mu$ is the chemical potential and we work in the grand canonical ensemble. In the present study we consider an attractive interaction, $U < 0$. The Hamiltonian of Eq. (1) has been studied in detail by Micnas et al \cite{Micnas}.

Nolting \cite{Nolting} and Kalashnikov and Fradkin \cite{Kalashnikov} have derived exact relations for the one-particle spectral functions, $A(k, \omega)$ and $B(k, \omega)$, which are given by:

$$M^{(0)}(k) \equiv \int_{-\infty}^{+\infty} A(k, \omega) d\omega = 1 ,$$

$$M^{(1)}(k) \equiv a_1 \equiv \int_{-\infty}^{+\infty} \omega A(k, \omega) d\omega = \varepsilon_k - \mu + \rho U ,$$

$$M^{(2)}(k) \equiv a_2 \equiv \int_{-\infty}^{+\infty} \omega^2 A(k, \omega) d\omega = (\varepsilon_k - \mu)^2 + 2\rho(\varepsilon_k - \mu)U + \rho U^2 ,$$
where \( \epsilon(k) = -2t(\cos(k_x a) + \cos(k_y a)) \), with \( a \) the lattice constant. \( \Delta_o(T) \), the off-diagonal long range order, and \( \rho \), the carrier concentration per spin, \( n/2 \), have to be calculated self-consistently. \( A(k, \omega) \) and \( B(k, \omega) \) are the diagonal and off-diagonal one-particle spectral functions, respectively. They are defined by:

\[
\begin{align*}
A(k, \omega) &\equiv -\frac{1}{\pi} \lim_{\delta \to 0^+} Im[G(k, \omega + i\delta)] ; \\
B(k, \omega) &\equiv -\frac{1}{\pi} \lim_{\delta \to 0^+} Im[F(k, \omega + i\delta)] .
\end{align*}
\]

The parameter \( B_\sigma \), the Nolting’s approximation, is given in a self-consistent way. \( \rho \) and \( \Delta_o(T) \) are calculated from

\[
\rho = \frac{1}{N} \sum_k \int_{-\infty}^{+\infty} d\omega \frac{A(k, \omega)}{e^\beta \omega + 1} ; \quad \Delta_o(T) = \frac{1}{N} \sum_k \int_{-\infty}^{+\infty} B(k, \omega) \frac{1}{e^\beta \omega + 1} .
\]

The main ingredient in any correct description of a physical system is the availability of the one-particle Green’s function. Of course, in a many-body problem we cannot have a closed expression. In order to show the way, we first discuss the 2D BCS case in the framework of the moment approach and then we study the case of superconductivity beyond BCS, i.e., by including higher order moments. Here one must note that due to the Mermin-Wagner theorem no phase-transition is expected in 2D in systems with a continuous symmetry, and the formalism here is too simple to describe a Kosterlitz-Thouless phase-transition. Nonetheless, it is observed that the formalism does give a phase-transition.

**A. BCS case**

Let us postulate as our one-particle spectral functions the following ones:

\[
\begin{align*}
A(k, \omega) &= \alpha_1(k) \delta(\omega - E_k) + \alpha_2(k) \delta(\omega + E_k) \quad , \quad (10) \\
B(k, \omega) &= \sqrt{\alpha_1(k) \alpha_2(k)} \left[ \delta(\omega - E_k) - \delta(\omega + E_k) \right] \quad , \quad (11)
\end{align*}
\]

By using this Ansatz in the moment equations, we obtain that:

\[
E_k = \sqrt{\left( \epsilon_k - \mu + \rho U \right)^2 + \Delta_o^2(T)} ; \quad \alpha_1(k) = \frac{1}{2} \left( 1 + \frac{\epsilon_k - \mu + \rho U}{E_k} \right) ; \quad \alpha_2(k) = 1 - \alpha_1(k) . \quad (12)
\]

Eqs.(12) are clearly the BCS solutions with the Hartree shift, \( \rho U \), included in a natural way. The quasi-particle excitation spectrum, \( E_k \), has been obtained from the particular form of the off-diagonal single-particle spectral function, i.e., the square root dependence. This square root dependence will be kept when we include correlations, i.e., when we include higher order moments, i.e., \( a_2 \) and \( a_3 \). This we will do next.

**B. Correlations on the BCS solution.**

Now, we will go beyond the BCS solution by including correlations in higher order. In this case, the physical picture is that superconductivity is similar to BCS in the sense that we will have quasi-particle spectra with a gap around the chemical potential.

In order to keep the picture simple, we will assume that the chemical potential, \( \mu \), is close to the bottom of the free band. Then, the superconducting gap opens up around the chemical potential and there is an upper Hubbard band which remains almost similar to the Hubbard band when the order parameter is zero, i.e., when there is no
symmetry breaking. In this case, we postulate that the diagonal one-particle spectral density is composed of three poles as follows:

\[ A(k, \omega) = \alpha_1(k)\delta(\omega - \hat{\Omega}_1(k)) + \alpha_2(k)\delta(\omega - \hat{\Omega}_2(k)) + \alpha_3(k)\delta(\omega - \hat{\Omega}_3(k)) \]  

In Eq. (13), the first two poles represent the behavior around the chemical potential and the third pole is due to the influence of the upper Hubbard band, which in the case of the atomic limit, \( t = 0 \), is the upper Hubbard band or the band of single occupied states. The lower band, now split in two, is the band of doubly occupied states for the case of almost atomic limit. The off-diagonal (anomalous) spectral function has the same form given as in the BCS case. Of course, our parameters \( \alpha_j(k) \) and \( \hat{\Omega}_j(k) \) have to be calculated self-consistently (\( \hat{\Omega}_1(k) = +E_k; \hat{\Omega}_2(k) = -E_k; \hat{\Omega}_3(k) = \Omega_k \)). Now, the parameter \( B_\sigma \) which appears in \( a_3(k) \) is generally \( k \)-dependent. In the spherical approximation, it is \( k \)-independent and is calculated from the following equation:

\[ \rho(1 - \rho)B_\sigma = \frac{1}{N} \sum_k \sum_{j=1}^3 \alpha_j(k)\varepsilon_k \frac{1}{e^{\beta\hat{\Omega}_j(k)} + 1} \left[ \frac{2}{U} (\hat{\Omega}_j(k) + \mu - \varepsilon_k) - 1 \right] , \]  

where \( \beta = 1/(k_BT) \), \( T \) the absolute temperature, \( k_B \) the Boltzmann’s constant, and \( N \) the number of lattice sites. Next, by putting our ansatz \( A(k, \omega) \) and \( B(k, \omega) \) into the set of moment equations, we get to lowest order in \( \Delta_\sigma^2 \)

\[ \alpha_1(k) = \frac{1}{2} \left( \frac{\Omega_k - a_1(k)}{\Omega_k - H_k} \right) \left[ 1 + \frac{H_k}{E_k} \right] ; \quad \alpha_2(k) = \frac{1}{2} \left( \frac{\Omega_k - a_1(k)}{\Omega_k - H_k} \right) \left[ 1 - \frac{H_k}{E_k} \right] ; \quad \alpha_3(k) = 1 - \alpha_1(k) - \alpha_2(k) , \]  

where the quasi-particle energy is given by

\[ E_k = \sqrt{H_k^2 + \left( \frac{\Omega_k - H_k}{\Omega_k - a_1(k)} \right)^2 \Delta_\sigma^2(T)} \]  

with

\[ H_k \approx H_o(k) = \Omega_1(k) = \frac{1}{2} \left[ \varepsilon_k - 2\mu + U + B - \sqrt{(\varepsilon_k - U - B)^2 + 4\rho U(\varepsilon_k - B)} \right] \]

\[ \Omega_k \approx \Omega_o(k) = \Omega_2(k) = \frac{1}{2} \left[ \varepsilon_k - 2\mu + U + B + \sqrt{(\varepsilon_k - U - B)^2 + 4\rho U(\varepsilon_k - B)} \right] , \]  

where the \( \Omega_j(k) \)’s are the ones which enter in the moment equations in the normal state (Eqs. (17) and Ref. [7]). However, due to the fact that the narrowing factor, \( B \), is a sum over three frequencies of our problem (see Eq. (14)) then all three parameters \( (\mu, B \text{ and } \Delta(T)) \) are mixed together.

From Eqs. (16,17) we see that the quasi-particle energy, \( E_k \), has a gap which we find to be:

\[ \Delta(T, k) = \Delta_o(T) \left( \frac{\Omega_2(k) - \Omega_1(k)}{\Omega_2(k) - a_1(k)} \right) \]  

From Eq. (18) we conclude that our gap equation, which is a manifestation of singularities in the density of states, is \( k \)-dependent. Going back to our local Hamiltonian (see Eq. (1)), which in reciprocal space is a constant, then at the mean field level we should obtain a pure \( s \)-wave, while going beyond mean field approximation we have been able to derive a \( k \)-dependent gap. In our case, we have been able to modify the BCS results, from pure \( s \)-wave to a wave vector dependent energy gap.

Our Ansatz is based on the assumption that the role of correlations is mainly taken into account in the diagonal one-particle spectral function. This implies that the off-diagonal order parameter has been taken to as the BCS one, i.e., to \( m^{(1)}(k) \). In a previous work, [14] it is found that both the diagonal and off-diagonal spectral functions have four peaks, symmetric in pairs, for \( U/t = -4 \). However, in the diagonal spectral function the fourth peak has a small weight and it is neglected here. If we want to consider two other peaks for the off-diagonal spectral function we have to include more moments, which is beyond the present work. Also, we have neglected life-time effects in Eq. (13), which would require the evaluation of higher moments. We leave this out from the present calculation.

In Fig. 1 we show the dependence of the reduced gap as function of reduced temperature. For comparison, we have also included the BCS gap. The critical temperature, \( T_c/\mu \), has the value 0.80 and the gap at zero temperature is 0.66\( \mu \). Then, for the ratio \( \Delta(0)/T_c \) we find 0.825. We should compare this with the BCS universal value, 1.76, for the same parameters [11 - 14]. In Fig. 2 we show the energy spectra for the three bands involved in the diagonal spectral
density. We observe that the third band, $\Omega_k$, is almost always on top of the superconducting bands, i.e., $\pm E_k$. In the inset of Fig. 2 we include a blowup of $E_k$ close to its minimum, in order to calculate the gap. In Fig. 3 we present the $k$ dependent factors, $\gamma_1(k)$ and $\gamma_2(k)$,

$$\gamma_1(k) = \frac{(\Omega_2(k) - \Omega_1(k))\Delta_o^2(T)}{(\Omega_2(k) - a_1(k)a_2(k))}, \quad \gamma_2(k) = \frac{(\Omega_2(k) - \Omega_1(k))\Omega_1(k)\Delta_o^2(T)}{(\Omega_2(k) - a_1(k)a_3(k))},$$

for $T/t = 0.001, U/t = -4.0$ and $\rho = 0.1$. These factors, which represent a correction to our frequencies, $H_k$ and $\Omega_k$, are zero at $T_c$. This implies that they do not change the value of $T_c$. However, for $T \approx 0$ they reach up to $0.25$. This contribution may look small but we have to remember that our equations are highly non-linear and a small change could produce a large change in the variables of interest, i.e., $\Delta(0)$. In consequence, our results support the calculations of Refs. [11]-[12] in the sense that the critical temperature is renormalized by more than a factor of two with respect to the BCS value. On the other hand, we argue that the value of the gap at zero temperature is going to be modified by the inclusion of the $\gamma(k)$’s, which are going to increase the value of $\Delta(0)$. Due to these arguments, our calculation is of a perturbative character in $\Delta_o^2(T)$. In the calculation of Pedersen et al [10] the authors find a critical temperature of $T_c = 0.19$ by using a different moment approach where the spectral functions have four peaks. Our calculations for the spectral weight supports the view of ref [10] because there is an additional band which splits off from $\alpha_3(k)$. [13] The appearance of a fourth band will modify the value of $T_c$ and also the value of the gap. However, the numerical $T_c/t$ in the present work is different than the one given in ref. [10].

By using the moment approach in the presence of off-diagonal long range order, i.e., $\Delta_o(T) \neq 0$, to the negative Hubbard model, we have worked out the attractive Hubbard model in 2-D with an ansatz where the diagonal spectral function has three peaks and the off-diagonal one has two. The physical meaning of each of these peaks has been discussed. We have solved our equations in lowest order of $\Delta_o(T)$, an approximation which obviously is valid close to $T_c$ but it fails for zero temperature. We have seen that the effect of the third band is to renormalize the order parameter producing an energy gap which is $k$-dependent. In consequence, in our approach the order parameter, $\Delta_o(T)$, and the energy gap, $\Delta(T, k)$, are not the same. A similar discussion was presented by Randeria, Duan and Shieh [4]. The implications of this point is that we can shed light on the experiments carried out in the high-temperature superconductor materials since the experimentalists are talking about the symmetry of the order parameter and from the theoretical side we should refer to the energy gap. These two concepts are valid in mean field theory, i.e., in the BCS approximation. When we go beyond BCS as in the present work, it is difficult to assess the symmetry of the order parameter from tunelling experiments only. Then, from the experimental side it is difficult to find the symmetry of the order parameter unless the high temperature superconductors obey mean field equations. In short, the messages of this paper are

- **1-** Due to correlations, the order parameter and the gap are two different quantities. In our case, from a local pairing attraction, i.e., pure s-wave in mean field, we get a $k$ gap function.

- **2-** Our calculations are of a perturbative character and they agree with Refs. [11]-[12]. Work is in progress [13] to include additional bands in the diagonal spectral function. This will be published elsewhere.

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Figures.

Fig. 1.- The energy reduced gap, $\Delta(T)/\Delta(0)$, as function of reduced temperature, $T/T_c$, for $U/t = -4.0$, $\rho = 0.1$. See Fig. 2 (inset) for the definition of $\Delta(T)$.

Fig. 2.- The energy bands, $\pm E_k$ and $\Omega_k$ along the diagonal of the Brillouin zone. For comparison, we have included the BCS energy bands. In the inset we have made a blow up of $+E_k$ close to the minimum of the band. This allows us to find $\Delta(T)$. Same parameters as in Fig. 1 with $T/t = 0.001$.

Fig. 3.- We plot $\gamma_1, \gamma_2$ vs k, along the diagonal of the Brillouin zone for the same parameters in Fig. 2. The parameters $\gamma$’s are defined in Eq. (19).
Fig. 1

\[ \frac{\Delta(T)}{\Delta(0)} \]

vs.

\[ \frac{T}{T_C} \]
