Investigation of BCS gap equation of (d+id) hole doped cuprates

Partha Goswami
Physics Department, D.B.College(University of Delhi),Kalkaji,Delhi-110019, India

physicsgoswami@gmail.com

Abstract. We consider a (d + i d) cuprate superconductor and model the functional dependence of the pairing interactions $V(k,k') = (V_{x^2-y^2}(k,k') + V_{xy}(k,k'))$ required for d+id ordering in the pseudo-gap (PG) phase by a function of the form $V_{\text{trial}} = (V_{x^2-y^2}(k_F,k_F) + V_{xy}(k_F,k_F)) F(\phi,\phi')$, where $V_{x^2-y^2}(k,k') = V_1 (\cos k_x a - \cos k_y a) \cos k'_x a - \cos k'_y a$, $V_{xy}(k,k') = V_2 \sin k_x a \sin k_y a \sin k'_x a \sin k'_y a$, $V_1$ and $V_2 (V_1 > V_2)$ are the coupling strengths, $k_F$ is the Fermi momentum, $\phi = \text{arc}(\tan(k_y/k_x))$, and $(k_x,k_y)$ belong to the first Brillouin zone (BZ). We further assume that an attractive interaction $-|U_1| (\cos k_x a - \cos k_y a) \cos k'_x a - \cos k'_y a$, where $U_1$ is a model parameter, is responsible for d-wave superconductivity (DSC). Within the BCS framework, for $V_2 << V_1$, we show that the resultant zero-temperature gap $\Delta_0(0)$ is an increasing function of $g(k_F || (\mathbf{D}/2)) (|U_1| + V_1)$ where the quantity $\mathbf{D}$ is the density of energy states). The solutions are possible if $|U_1| = V_1$. The exercise underscores the fact that the unconventional superconductivity in the hole-doped cuprates may definitely be described within the BCS framework.

1. Introduction

The high temperature superconductivity in hole-doped cuprates, such as YBa$_2$Cu$_3$O$_{7-\delta}$, is derived by doping the parent two-dimensional Mott insulators with a large antiferromagnetic exchange interaction. It is now an established view [1] that the superconducting (SC) gap in such systems have robust d-wave symmetry while the pseudo-gap (PG) is of d+id variety [2,3]. The under-doped metallic region between 0.10 $\leq \delta \leq 0.16$ for this system has attracted much attention because of the anomalous temperature dependence (a non-Fermi liquid behavior) of the electronic specific heat, the magnetic susceptibility, etc.. In YBa$_2$Cu$_3$O$_{7-\delta}$, upon hole doping, the anti-ferromagnetism is destroyed at the hole density $\delta \sim 0.10$ and the superconductivity is optimized at $\delta \sim 0.16$. Further doping leads to decreasing $T_c$ and more or less conventional Fermi-liquid behavior. Regarding the origin of the PG and its relation with superconductivity (SC), however, there are two different views. In one, the PG is regarded as a superconducting precursor state (SPS) involving incoherent electron-electron pairings above $T_c$ [4,5,6,7,8,9] with the particle-hole symmetry preserved whereas the other regard the PG, distinct from SC, to be an ordered state with particle-hole asymmetry and both the phases compete[10,11,12,13]. Chakravarty et al[11] had put forward interpretation of this gap in terms of a hidden long-range order, viz. d-density wave (DDW) order which corresponds to spontaneous currents along the bonds of a square lattice for the ordering wave vector $\mathbf{Q} = (\pm \pi, \pm \pi)$. Although the currents violate the microscopic time reversal symmetry
(MTRS), there is no macroscopic violation. This happens as the DDW state preserves the combined effect of MTRS and translation by a lattice spacing. The net result is that the staggered magnetic flux produced by these currents is zero on the macroscopic scale. Our view regarding the origin of the PG is, however, centered around the paradigm that PG corresponds to d+id-density wave (chiral DDW or CDDW) ordering [2, 3] at the anti-ferromagnetic wave vector \( \mathbf{Q} = (\pi, \pi) \). Many theorists and experimentalists subscribe to this view [2, 3, 14]. Accordingly, we model the effective fermion pairing interaction \( V(\mathbf{k}, \mathbf{k'}) \) in the singlet pairing channel by suitable function of the form \( V_{\text{trial}} = [(V_{x^2−y^2}(k_F, k_F) + V_{xy}(k_F, k_F)) F(\phi, \phi')] \), where \( V_{x^2−y^2}(\mathbf{k}, \mathbf{k'}) = V_1(\cos k_x a−\cos k_y a) \cos k'_x a−\cos k'_y a, \) \( V_{xy}(k, k') = V_2 \sin (k_x a) \sin (k_y a) \sin (k'_x a) \sin (k'_y a) \), \( V_1 \) and \( V_2 \) are the coupling strengths, \( k_F \) is the Fermi momentum, \( \phi = \arctan(k_y / k_x) \), and \( (k_x, k_y) \) belong to the first Brillouin zone (BZ). As regards d-wave superconductivity (DSC), we model the effective two-particle pairing interaction \( U(\mathbf{k}, \mathbf{k'}) \) in the singlet pairing channel by suitable function of the form \( U(\mathbf{k}, \mathbf{k'}) = U_1 \cos k_x a−\cos k_y a \) \( \cos k'_x a−\cos k'_y a \) where \( U_1 \) is the coupling strength (model parameter). We assume implicitly that this unconventional superconductivity is initiated by the strongly coupled bosonic modes, such as those corresponding to the electron spin fluctuations (proximity to an anti-ferromagnetic phase raises the possibility of spin-fluctuation-mediated pairing).

In our scheme the Fermi level is pinned at the Van Hove singularity [15] of the normal state dispersion \( \epsilon_{k} \) involving the first, the second, and the third neighbor hopping plus a constant term. All energies are expressed in units of the first neighbor hopping. With all these paraphernalia, there are only two energy gaps \( \Delta_{k} = (−\epsilon_{k}+i\Delta_{k}) \) and \( \Delta_{k}^{(sc)} \) corresponding to PG and DSC, respectively, and two distinct quasi-particle dynamics in our formulation of the problem. The second-neighbor hopping in the dispersion, which is known to be important for cuprates [16] and frustrates the kinetic energy of electrons, leads to Fermi surface sheets being not connected by \( \mathbf{Q} = (\pi, \pi) \) (non-nesting property). One will notice that, the two gaps in the excitation spectrum are distinct and do not merge into one `quadrature' gap \( \Delta_{k}^{(eff)} = (1 / D_{k}^{2} + \Delta_{k}^{(sc)})^{2} \) if the nesting property, \( \epsilon_{k} = −\epsilon_{k+Q} \), of the dispersion is absent. We have solved the coupled equations for \( (D_{k}, D_{k}^\dagger) \) and \( \Delta_{k}^{(sc)} \) assuming \( V_2 \ll V_1 \) and the specific form for the interactions \( U(\mathbf{k}, \mathbf{k'}) \) and \( V(\mathbf{k}, \mathbf{k'}) \) given above together with the equation to determine the chemical potential \( \mu \) obtainable from the Luttinger rule. The noteworthy outcome of the exercise is the condition \( |U_1| \approx V_1 \) for the superconductivity in the hole-doped cuprates. Since \( V_1 \) has the coulombic origin [11], the superconductivity in the hole-doped cuprates is likely to have the same origin.

In the present communication we derive (see section 2) an expression for single-particle excitation spectrum in CDDW+DSC state. In section 3 we set up the equations for \( D_{k}, D_{k}^\dagger \) and \( \Delta_{k}^{(sc)} \). We solve these equations together with the equation to determine the chemical potential \( \mu \) of the fermion number in a sample case. All the numerical values are expressed in the units of the first neighbor hopping. We show in section 4 that the gap equations have reasonable solutions within the BCS framework even for the unconventional superconductivity.

2. CDDW Hamiltonian and single-particle excitation spectrum
We consider the usual\cite{2,3,11} tight-binding energy dispersion $\varepsilon_k = \varepsilon_k^{(1)} + \varepsilon_k^{(2)} + \varepsilon_k^{(3)} + 4t^\prime$, $\varepsilon_k^{(1)} = -2t(c_x + c_y)$, $\varepsilon_k^{(2)} = 4t^\prime c_x c_y$, $\varepsilon_k^{(3)} = -2t^\prime(c_x' + c_y')$. $c_{j} = \cos k_{ja}$, $c_{j}' = \cos 2k_{ja}$ ($j = x,y$), and a' is the lattice constant. The quantity $\varepsilon_k$ involves $t$, $t^\prime$, $t^\prime'$ which are the hopping elements between nearest, next-nearest (NN) and NNN neighbors, respectively. The energy $\varepsilon^{(1)}(k)$ satisfies the perfect nesting condition $\varepsilon^{(1)}(k+Q) = -\varepsilon^{(1)}(k)$ with anti-ferromagnetic wave vector $Q = (\pm \pi, \pm \pi)$. For the hole-doped materials, $t^\prime > 0$ (for the electron-doped materials $t^\prime < 0$), and, in all cases, $t^\prime < (t/2)$. For example, typical values are $t \sim 0.2$ eV, $(t^\prime/t) \sim 0.4$, and $(t^\prime'/t) \sim 0.01$\cite{15}. In the second-quantized notation, the Hamiltonian to deal with the d+id density-wave (CDDW) order at the wave vector $Q$ plus the d-wave superconductivity can be expressed as

$$H = \sum_{k,\sigma} \varepsilon_k d_{k,\sigma}^\dagger d_{k,\sigma} + \sum_{k,\sigma} \varepsilon_{k+Q} d_{k+Q,\sigma}^\dagger d_{k,\sigma} + \sum_{k,\sigma} \Delta_k d_{-k^\prime,-\sigma}^\dagger d_{k,\sigma} + \sum_{k,\sigma} \Delta_k^{sc} d_{k,\sigma}^\dagger d_{-k,-\sigma}^\dagger$$

(1)

where $D_k = (-\gamma_k + i\Delta_k) \equiv -\sum_{k,\sigma} V(k,\kappa') \cdot d_{k',\sigma}^\dagger d_{k,\sigma}^\dagger$ and $D_k^\dagger = (-\gamma_k - i\Delta_k) \equiv -\sum_{k,\sigma} V(k,\kappa') \cdot d_{k',\sigma} d_{k,\sigma}$. The gap function $\Delta_k^{sc} \equiv \sum_{k,\sigma} U(k,\kappa') d_{k,\sigma}^\dagger d_{-k,-\sigma} = -\Delta_k^{sc}(\kappa')$. In (1), $d_{k,\sigma}$ with $\sigma = \pm 1$, corresponds to the fermion annihilation operator for the single-particle state $(k,\sigma)$. In the pure d-wave case, $\Delta_k^{sc} = \Delta_k^{sc}(x) = (\Delta_0^{sc}(T))(\cos k_{xa} - \cos k_{ya})$. The quantities $(\gamma_k, \Delta_k)$ are given by $\gamma_k = -\gamma_0 \sin(k_{xa}) \sin(k_{ya})$, and $\Delta_k = (\Delta_0^{sc}(T))(\cos k_{xa} - \cos k_{ya})$. The conical brackets stand for the thermal average calculated with $H - \mu \tilde{N}$ where $\mu$ is the chemical potential of the fermion number, and $\tilde{N}$ is the total number operator. Upon ignoring the third neighbor hopping term in the dispersion $\varepsilon_k$ above, we find that the dispersion typically has two in-equivalent saddle points (van Hove singularities (vHs)) at $(\pi,0)$ and $(0,\pi)$ in the first Brillouin Zone. Upon assuming that for fillings such that the Fermi curve lies close to the singularities, the majority of states participating in the pairing formation will come from regions in the vicinity of these saddle points. It must be noted that the CDDW + DSC ordering leads to pining of the Fermi level close to, but not precisely at the vHs.

At this point we introduce few thermal averages determined by $H - \mu \tilde{N}$, viz. $G_\sigma(k,\tau) = -\langle \{ d_{k,\sigma}(\tau) d_{k,\sigma}(0) \} \rangle$, $\Gamma_\sigma(k,\tau) = -\langle \{ d_{k,\sigma}^\dagger(\tau) d_{k,\sigma}(0) \} \rangle$, $G_\sigma(k,\tau) = -\langle \{ d_{k+Q,\sigma}(\tau) d_{k,\sigma}^\dagger(0) \} \rangle$, $\Gamma_\sigma(k,\tau) = -\langle \{ d_{k+Q,\sigma}^\dagger(\tau) d_{k,\sigma}(0) \} \rangle$, and $G_\sigma(k,\tau) = -\langle \{ d_{k,\sigma}(\tau) d_{k+Q,\sigma}(0) \} \rangle$. Here $T$ is the time-ordering operator which arranges other operators from right to left in the ascending order of imaginary time $\tau$. The first step of the scheme involves the calculation of (imaginary) time evolution of the operators $d_{k,\sigma}(\tau)$ where, in units such that $h = 1$, $d_{k,\sigma}(\tau) = \exp(\mathcal{H} \tau) d_{k,\sigma}(0) \exp(-\mathcal{H} \tau)$. We obtain, for example, $\partial \tau \{ d_{k,\sigma}^\dagger(\tau) (\mathcal{H} d_{k,\sigma}(\tau) + \Delta_k^{sc} d_{k,\sigma}^\dagger d_{-k,-\sigma} + D_k^\dagger d_{-k,Q,\sigma}) \}$. Here $\partial \tau \equiv (\partial/\partial \tau)$ and the argument part has been dropped in writing the operators $d_{k,\sigma}(\tau)$ and their derivative. As the next step, we find that the equations of motion of the averages are given by

$$\partial G_\sigma(k,\tau) = -\langle \varepsilon_k - \mu \rangle G_\sigma(k,\tau) - \Delta_k^{sc} \Gamma_\sigma(k,\tau) - D_k G_\sigma(k,\tau) - \delta(\tau),$$

$$\partial \Gamma_\sigma(k,\tau) = \langle \varepsilon_k - \mu \rangle \Gamma_\sigma(k,\tau) - \Delta_k^{sc} G_\sigma(k,\tau) + D_k^\dagger \Gamma_\sigma(k,\tau),$$

$$\partial G_\sigma(k,\tau) = -\langle \varepsilon_{k+Q} - \mu \rangle G_\sigma(k,\tau) - D_k G_\sigma(k,\tau) + \Delta_k^{sc} \Gamma_\sigma(k,\tau).$$
\[ \partial \Gamma_{\sigma} (k, \tau) = (\varepsilon_k + \mu - \mu) \Gamma_{\sigma} (k, \tau) + D_k \Delta_k (sc) G_{\sigma} (k, \tau) + \Delta_k (sc) G_{\sigma} (k, \tau). \] (2)

The final step is the calculation of the Fourier coefficients \( G_{\sigma} (k, \omega_n) = e^{i \omega_n \tau} G_{\sigma} (k, \tau) \) (where the Matsubara frequencies are \( \omega_n = [(2n+1)\pi / \beta] \) with \( n = 0, \pm 1, \pm 2, \ldots \)) of these temperature Green’s functions. Here \( \beta = (k_B T)^{-1} \). We refrain from writing explicitly the equations to determine these coefficients as this is a trivial exercise in view of (2). Upon solving the equations we obtain \( G_{\sigma} (k, \omega_n) = (\Delta_{1/\Delta}), \Gamma_{\sigma} (k, \omega_n) = (\Delta_{2/\Delta}), G'_{\sigma} (k, \omega_n) = (\Delta_{3/\Delta}), G''_{\sigma} (k, \omega_n) = (\Delta_{4/\Delta}) \) where

\[ \Delta = (i \omega_n)^4 - (i \omega_n)^2 (\xi_k^2 - 2 \xi_{k+Q}^2 + 2 D_{eff} (k)^2) + \frac{\xi_k + \xi_{k+Q}^2}{2} - 2 \xi_k \xi_{k+Q} |D_k|^2 + \Delta_k (sc)^2 (\xi_k^2 + 2 \xi_{k+Q}^2) \]

\[ + \frac{\Delta_k (sc)^4 + |D_k|^2 - |D_k|^2 \Delta_k (sc)^2 - |D_k|^2 \Delta_k (sc)^2}{2}, \]

\[ \Delta_1 = (i \omega_n + \xi_k) ((i \omega_n)^2 - \xi_{k+Q}^2 - \Delta_k (sc)^2) - |D_k|^2 (i \omega_n - \xi_{k+Q}), \]

\[ \Delta_2 = \frac{\Delta_k (sc)^4 (i \omega_n)^2 - \xi_{k+Q}^2 - \Delta_k (sc)^2 - |D_k|^2 (i \omega_n - \xi_{k+Q})}{2}, \]

\[ \Delta_3 = D_k (i \omega_n + \xi_k) (i \omega_n + \xi_{k+Q}) - D_k (-\Delta_k (sc)^2 + |D_k|^2), \]

\[ \Delta_4 = D_k (i \omega_n + \xi_k) (i \omega_n + \xi_{k+Q}) + D_k \Delta_k (sc) (i \omega_n - \xi_{k+Q}), \]

\[ \Delta_5 = D_k (i \omega_n + \xi_k) (i \omega_n + \xi_{k+Q}) - D_k (-\Delta_k (sc)^2 + |D_k|^2), \]

\[ (3) \]

\( \xi_k = \varepsilon_k - \mu \), and \( D_{eff} (k)^2 = (|D_k|^2 + \Delta_k (sc)^2) \). The denominator \( \Delta \) of the Fourier coefficients yields the single particle excitation spectrum \( E_k (T>T_c) \): \( E_k (T<T_c) = \pm E_k^{(U,L)} (k) \). \( E_k^{(U,L)} \)

\[ = \frac{1}{2} ([\xi_k^2 + \xi_{k+Q}^2 + 2 D_{eff} (k)^2] \pm p(k)), \]

and \( p(k) = [(\xi_k^2 - \xi_{k+Q}^2)^2 + 4|D_k|^2 (\xi_k + \xi_{k+Q})^2 + 4(|D_k|^2)^2 + (|D_k|^2)^2 - 2 |D_k|^2 \Delta_k (sc)^2])^{1/2} \). The excitations in cuprates are thus demonstrably Bogoliubov quasi-particles in the DSC phase. One may notice that, the two gaps in the excitation spectrum are distinct and do not merge into one `quadrature’ gap \( (D_{eff} (k)^2 = |D_k|^2 + \Delta_k (sc)^2) \) even if the dispersion is nested \( (\varepsilon_k = -\varepsilon_{k+Q}) \). The reason being the complex d-wave order parameter \( D_k \) describing the PG state breaks the time-reversal symmetry of the normal state. The time-reversal operator \( \hat{O} \) transforms the order parameter to its complex conjugate: \( \hat{O} D_k = D_k^\dagger \). If the time-reversal symmetry is preserved, \( D_k \) and \( D_k^\dagger \) are identical to within a common spatially independent phase. If, however, the time-reversal symmetry is broken, the two states are distinct albeit with the same free energy. The bands \( E_k^{(U,L)} \) above the Fermi energy are the reflected ones of those below the Fermi energy, i.e. \( -E_k^{(U,L)} \). For \( V_2 << V_1 \) the band-maxima in \( E_k^{(U)} \) occur at the points \( (\pm \pi, \pm \pi) \) and \( (0,0) \) whereas those in \( E_k^{(L)} \) occur at the points \( (\pm \pi/2, \pm \pi/2) \). On the other hand, the band-minima in \( -E_k^{(U)} \) occur at the anti-nodal points \( (\pm \pi,0) \) and \( (0,\pm \pi) \) while the band-minima in \( -E_k^{(L)} \) occur at the nodal points \( (\pm \pi/2, \pm \pi/2) \). Since the Bogoliubov quasi-particles here with energy above the Fermi sea do not behave the same as those below the Fermi energy, we have clear particle-hole asymmetry in the CDDW+DSC state.

3. Equations for \( D_k, D_k^\dagger \) and \( \Delta_k (sc) \)

For the perfectly nested dispersion, since \( p(k) = 4i\Delta_k \Delta_k (sc) \), one may write the Fourier coefficient \( G_{\sigma} (k, \omega_n) \) as
\[
G_\sigma(k,\omega_n) = \sum_{j=\pm 1} \{ U^{(j)}_k (i\omega_n + j(\xi_k + i\xi^{-1}_k))^{-1} + V^{(j)}_k (i\omega_n + j(\xi_k - i\xi^{-1}_k))^{-1}\},
\]

(4a)

\[
\xi_k = R_k^{1/2}\cos(\theta_k/2), \quad i\xi^{-1}_k = R_k^{1/2}\sin(\theta_k/2), \quad R_k = [(\xi_k^2 + D_{\text{eff}}(k)^2)^2 + 4\Delta^2_k \Delta_k^{(sc)}]^{1/2},
\]

(4b)

\[
\tan^2(\theta_k) = \frac{(4\Delta^2_k \Delta_k^{(sc)})}{(\xi_k^2 + D_{\text{eff}}(k)^2)^2},
\]

(4c)

\[
U^{(j)}_k = (1/4)[1 - (j\xi_k/ R_k^{1/2}\exp(i\theta_k/2))], \quad V^{(j)}_k = (1/4)[1 - (j\xi_k/ R_k^{1/2}\exp(-i\theta_k/2))],
\]

(4d)

In (4d) we have used the fact that for the nested dispersion \(E_k^{(sc)} = [\xi_k^2 + D_{\text{eff}}(k)^2 \pm 2i\Delta_k \Delta_k^{(sc)}] \). The sum of the coherence factors \(\sum_{j=\pm 1} \{ U^{(j)}_k + V^{(j)}_k \} = 1 \) but the factors are complex unlike the usual Fermi liquid(FL) picture. We shall, however, presently focus our attention on the imperfect nesting (and when \(p(k) \) is likely to be real) and revisit the near-nested situation while seeking approximate solutions of the gap equations analytically in section 4. For the imperfect nesting case we have

\[
G_\sigma(k,\omega_n) = \sum_{j=\pm 1} \{ U^{(j)}_k (i\omega_n + jE_k^{(U)})^{-1} + V^{(j)}_k (i\omega_n + jE_k^{(L)})^{-1}\},
\]

(5a)

\[
u^{(j)}_k = (1/2)[(1-j\xi_k/E_k^{(U)}) \times [(E_k^{(U)^2} - \xi_k^2 q(k)) / q(k)] - (1 + j\xi_k/q) \times (|D_k|/q(k))],
\]

(5b)

\[
v^{(j)}_k = -(1/2)[(1-j\xi_k/E_k^{(L)}) \times [(E_k^{(L)^2} - \xi_k^2 q(k)) / q(k)] - (1 + j\xi_k/q) \times (|D_k|/q(k))],
\]

(5c)

where \(\xi_k^2 q(k) = (\xi_k^2 + \Delta_k^{(sc)}), and q(k) = (E_k^{(U)^2} - E_k^{(L)^2})\). We find that the coherence factors \(U^{(j)}_k \) and \(V^{(j)}_k \) satisfy the sum rule \(\sum_{j=\pm 1} \{ U^{(j)}_k + V^{(j)}_k \} = 1 \). The equation to determine the chemical potential(\(\mu\)), according to the Luttinger rule, is now given by

\[
(1+p) = (N_s/2)^{-1} \sum_{j=\pm 1} \{ U^{(j)}_k \times (\exp(-j\mu E_k^{(U)}) + 1)^{-1} + V^{(j)}_k \times (\exp(-j\mu E_k^{(L)}) + 1)^{-1} \}
\]

(6)

where \(p \) is the hole-doping level, and \(N_s \) is the number of unit cells in the \(k\)-space. The \(k\)-sums in these equations will get replaced by the integration \(\int \rho_{\text{Fermi}}(k) \, dk \) when \(\rho_{\text{Fermi}}(k) \) stands for the Fermi energy density of states (DOS). The dimensionless density of states \(\rho(k,\omega) \equiv (-1/2\pi^2\rho_0) \Im \mathcal{G}^{(R)}(k,\omega) \) (where we take a broad-bandwidth, say, \((10t_1) \sim 1.65 \, \text{eV} \) which gives \(\rho_0 = (10t_1)^{-1} \sim 0.6 \, \text{eV}^{-1} \)) while the single-particle spectral function in the spin-\(\sigma\) channel is given by \(A_{\sigma}(k,\omega) = (-\pi^{-1}) \Im \mathcal{G}^{(R)}(k,\omega) \) (where \(\mathcal{G}^{(R)}(k,\omega) \) is the retarded Green’s function given by \(\mathcal{G}^{(R)}(k,\omega) = -\int_{-\infty}^{\infty} \mathcal{G}(\omega') (\omega - \omega' + i0^+) \mathcal{G}^{(R)}(k,\omega') \) and \(\mathcal{G}(k,\omega) = (1/4) \{ G_0(k, z = i\omega_n) \mid z = \omega + i0^+ - G_0(k, z = i\omega_n) \mid z = \omega + i0^+ \} \). Upon using the result \((x \pm i0^+)^{-1} = [P(x^2) \pm (1/\pi) \pi \delta(x) \}}, where \(P \) represents a Cauchy’s principal value, the spectral function \(A(k,\omega) \) in the CDDW+DSC phase is given by a sum of \(\delta \) functions at the quasi-particle energies: \(A(k,\omega) = 2\pi \sum_{j=\pm 1} \{ U^{(j)}_k \delta(\omega + jE_k^{(U)}) + V^{(j)}_k \delta(\omega + jE_k^{(L)}) \}\). We simply replace the \(\delta \) functions by Lorentzians with an assumed intrinsic life-time broadening \((\gamma/t_1) \sim 0.1 \). Thus, from the expression for spectral density, putting \(\omega = 0 \), we obtain \(\rho_{\text{Fermi}}(k) = (1/2\pi\rho_0)\sum_{j=\pm 1} \{ U^{(j)}_k (\gamma/t_1) \times [E_k^{(U)^2} + (\gamma/t_1)^2]^{-1} + V^{(j)}_k (\gamma/t_1) \times [E_k^{(L)^2} + (\gamma/t_1)^2]^{-1} \} \).
This leads to the usual Fermi arc picture on the first Brillouin zone. We shall, however, approximate this by a constant in section 4 while seeking solutions of the gap equations analytically.

The remaining Fourier coefficients \( G'_\sigma(k,\omega_n) \) and \( \Gamma_\sigma(k,\omega_n) \) which correspond to the CDDW gap and the DSC gap, respectively, are given by

\[
G'_\sigma(k,\omega_n) = \sum_{j=\pm1}(-j/2E_k^{(U)})\times\{[D_k^\dagger(E_k^{(U)}) - j\xi_k]\times(E_k^{(U)} - j\xi_{k+Q}) - D_k(-\Delta_k^{(sc)} + (D_k^\dagger)^2)]/q(k)\]
\[
\times(\imath\omega_n + jE_k^{(U)})^{-1}
\]
\[
+ \sum_{j=\pm1}(j/2E_k^{(L)})\times\{[D_k^\dagger(E_k^{(L)} - j\xi_k]\times(E_k^{(L)} - j\xi_{k+Q}) - D_k(-\Delta_k^{(sc)} + (D_k^\dagger)^2)]/q(k)\]
\[
\times(\imath\omega_n + jE_k^{(L)})^{-1},
\]
\[
\Gamma_\sigma(k,\omega_n) = \sum_{j=\pm1}(-j\Delta_k^{(sc)}/2E_k^{(U)})(E_k^{(U)} - \xi_{k+Q}^2 - \Delta_k^{(sc)} + D_k^\dagger)^2)/q(k)(\omega_n+jE_k^{(U)})^{-1}
\]
\[
+ \sum_{j=\pm1}(j\Delta_k^{(sc)}/2E_k^{(L)})(E_k^{(L)} - \xi_{k+Q}^2 - \Delta_k^{(sc)} + (D_k^\dagger)^2)/q(k)(\omega_n+jE_k^{(L)})^{-1}.
\]

We note that the Fourier coefficient \( G'_\sigma(k,\omega_n) \) corresponds to \( D_k^\dagger \) while the the coefficient \( G'_\sigma(k,\omega_n) \) corresponds to \( D_k \). Upon replacing \( D_k \) and \( D_k^\dagger \) respectively, by \(-\chi_k + i\Delta_k \) and \(-\chi_k - i\Delta_k \), the three Fourier coefficients \( G'_\sigma(k,\omega_n) \), \( G'_\sigma(k,\omega_n) \) and \( \Gamma_\sigma(k,\omega_n) \) lead to the coupled equations for CDDW gaps (\( D_k^\dagger, D_k \)) and DSC gap (\( \Delta_k^{(sc)} \)). With \( G'_\sigma(k,\omega_n) \) and \( G'_\sigma(k,\omega_n) \), in view of the definitions \( D_k^\dagger \equiv -\sum_{k',\sigma}V(k,k')d_{k',\sigma}^\dagger \) and \( D_k \equiv \sum_{k',\sigma}V(k,k')d_{k',\sigma} \), in the zero-temperature limit, we obtain

\[
\chi_k = \sum_{k',\sigma}V(k,k')[\chi_{k'}(1 + a(k'))/[2(E_{k'}^{(U)} + E_{k'}^{(L)})]],
\]
\[
\Delta_k = \sum_{k',\sigma}V(k,k')[\Delta_{k'}(1 + b(k'))/[2(E_{k'}^{(U)} + E_{k'}^{(L)})]],
\]

while with \( \Gamma_\sigma(k,\omega_n) \) we obtain

\[
\Delta_k^{(sc)} = -\sum_{k',\sigma}U(k,k')[\Delta_{k'}^{(sc)}(1 + c(k'))/[2(E_{k'}^{(U)} + E_{k'}^{(L)})]],
\]

where \( a(k) \equiv (\xi_k^2 + |D_k|^2 - \Delta_k^{(sc)})/(E_k^{(U)} + E_k^{(L)}) \), \( b(k) \equiv (\xi_k^2 + |D_k|^2 + \Delta_k^{(sc)})/(E_k^{(U)} + E_k^{(L)}) \), and \( c(k) \equiv (\xi_k^2 + |D_k|^2 + \Delta_k^{(sc)})/(E_k^{(U)} + E_k^{(L)}) \). In the zero-temperature limit when \( \chi_k \ll \Delta_k \) (or \( V_1 >> V_2 \)) and the nesting of the Fermi surface is near-perfect, \( \Gamma \) may be written as \( \Delta_k \approx \frac{1}{2}\sum_{k',\sigma}V(k,k') \{\Delta_k'/(\xi_k^2 + \Delta_k' + \Delta_k^{(sc)})^{1/2}\} \). For \( V(k,k') \approx V_1 \) (cos \( k_xa - \cos k_xa \)) (cos \( k'_xa - \cos k'_xa \)), the equation assumes a simple form

\[
1 \approx (V_1/2)\sum\{\{cos k_xa - \cos k_xa\}^2/\{\xi_k^2 + (\Delta_0(PG)(0))^2 + \Delta_0^{(sc)}(0)^2\} (\cos k_xa - \cos k_xa)^2\}^{1/2}. \]
Equation (9), on the other hand, yields $\Delta_k^{(SC)} = -\left(\frac{1}{2}\right) \sum_{k',\sigma} U(k,k') \Delta_{k'}^{-1} \times [\sqrt{\xi_k^2 + \Delta_k^2} + \Delta_k^{(SC)^2}]^{-1}$ which is formally similar to the weak coupling BCS gap equation. With an appropriate attractive interactions $U(k,k') = -|U| (\cos k_a - \cos k_{a'}) (\cos k_{a'} - \cos k_a)$ where $U_1$ is the coupling strength, we find that the equation assumes a simple form

$$
1 = \left(|U|/2\right) \sum_k [ (\cos k_a - \cos k_{a'})^2 / (\xi_k^2 + (\xi_{k'}^2 + (\Delta_0^{(PG)}(T=0)^2 + \Delta_0^{(SC)}(T=0)^2) (\cos k_a - \cos k_{a'})^2)^{-1/2}] \right). \tag{10b}
$$

The approximate solutions of the Eqs.(10), once obtained, may be substituted in (8a) to obtain $\chi_0$. The gap trio thus obtained may constitute a good starting point for an iterative scheme to solve Eqs.(8) and (9). For example, for the doping level 9.94% and temperature $T= 60$ K, solving these equations simultaneously we have found $\mu/t = -0.0018$, $\Delta_0^{(PG)}(T=0)/t = 0.0240$, $\chi_0/t = 0.0005$ and $\Delta_0^{(SC)}(T=0)/t = 0.0150$ for $(t'/t) = 0.0005$.

### 4. Unconventional superconductivity and BCS framework

Upon combining the two gap equations given by (10), we obtain

$$
1 = \left(\frac{1}{2}\right) (|U| + V_1) \sum_k [ (\cos k_a - \cos k_{a'})^2 / (\xi_k^2 + (\Delta_0^{(PG)}(T=0)^2 + \Delta_0^{(SC)}(T=0)^2) (\cos k_a - \cos k_{a'})^2)^{-1/2}] \right). \tag{11}
$$

We also obtain $|U_1| \approx V_1$ as the sum $\sum_k [ (\cos k_a - \cos k_{a'})^2 / (\xi_k^2 + (\Delta_0^{(PG)}(T=0)^2 + \Delta_0^{(SC)}(T=0)^2) (\cos k_a - \cos k_{a'})^2)^{-1/2}] \approx 0$. Since $V_1$ has its origin in the coulombic interaction[9], the condition $|U_1| \approx V_1$ obtained hints at the possibility of the superconductivity in the hole-doped cuprates initiated by the same interaction. Upon modeling the functional dependence of the pairing interactions and order parameter as $U(k,k') \rightarrow -|U| (\cos 2\varphi) \cos 2\varphi$, $V(k,k') \rightarrow V_1 \cos 2\varphi \cos 2\varphi$, and squared order parameter $\Delta_k(T=0)^2 = (\Delta_0^{(PG)}(T=0)^2 + \Delta_0^{(SC)}(T=0)^2) (\cos k_a - \cos k_{a'})^2 \rightarrow \Delta_0(T=0)^2 \cos^2 2\varphi$, where $\varphi \equiv \arctan (k_c/k_a)$ and $(k_c,k_y)$ belong to the first Brillouin zone (BZ), we may write the gap equation (11) as

$$
1 \approx g(k_F) \int [2\pi(\varphi/2\pi)] \times \int [\xi^2 + (\Delta_0(0)/\hbar\omega_c)^2 \cos^2 2\varphi)]
$$

$$
= g(k_F) \int [2\pi(\varphi/2\pi)] \cos^2 2\varphi \times \log [ (\Delta_0(0)/\hbar\omega_c)^2 \cos^2 2\varphi + 1 ]
$$

$$
/ (\Delta_0(0)/\hbar\omega_c) \times \cos 2\varphi) \right) \tag{12}
$$

where the dimensionless quantity $g(k_F) = \left(\frac{D}{2}\right) (|U_1| + V_1) \Delta_0(T=0)^2 + \Delta_0^{(SC)}(T=0)^2$ and we have assumed an arbitrary energy cut-off $\hbar\omega_c$ less than the Fermi energy. This facilitates integration over a length larger than $k_F^{-1}$. The quantity $\Delta_0$ with dimensions (Energy)$^{-1}$ which will be assumed to be a constant, is the density of energy states. In the weak coupling limit $g(k_F) \ll 1$, for the special situation $\varphi \rightarrow 0$, we obtain $(\Delta_0(0)/\hbar\omega_c) \approx 2 \exp(-1/g(k_F))$. This is reminiscent of the corresponding result of the BCS theory for the 'conventional superconductors'.
For the general situation, we adopt the simple strategy of assigning numerical values to \((\Delta_0(0)/\hbar \omega_c)\) and performing the integration in (12), by discretizing the integral, to obtain \(g(k_F)\). The 2-D graph in Figure 1 displays the outcome. We find that the quantity \((\Delta_0(0)/\hbar \omega_c)\) is an increasing function of \(g(k_F)\). Now at all temperatures above \(T = 0\) K, there is a finite possibility of finding electrons in the non-superconducting state. At finite temperature the occupation of the excited one electron state \(E_k = \sqrt{\xi^2 + (\Delta_k(T)/\hbar \omega_c)^2 \cos^2(2\phi)}\) obeys the Fermi statistics with the Fermi distribution \((\exp\beta E_k + 1)^{-1}\). Equation (12) is therefore replaced by

\[1 \approx g(k_F) \int_0^{2\pi} (d\phi/2\pi) \times \int_0^1 d\xi \left[ \cos^2(2\phi) / \sqrt{\xi^2 + (\Delta_0(0)/\hbar \omega_c)^2 \cos^2(2\phi)} \right] \times (1 - 2 f(T, \xi, (\Delta_0(0)/\hbar \omega_c), \phi)) \]  

(13)

where \(f(T, \xi, (\Delta_0(0)/\hbar \omega_c), \phi)\) = \((\exp\beta\hbar \omega_c \sqrt{\xi^2 + (\Delta_0(0)/\hbar \omega_c)^2 \cos^2(2\phi)})) + 1)^{-1}\). We assume that \(\Delta_0(T=0)^2 = (\Delta_0^{(PO)}(T=0)^2 + \Delta_0^{(SC)}(T=0)^2) \approx \Delta_0^{(SC)}(T=0)^2\). In that case one may say that the factor of 2 multiplying the Fermi function appears because either one of the states \(k\) or \(-k\) may be occupied. One can derive the equation for the critical temperature \(T_c\) readily from above:

\[2 = g(k_F) \int_0^1 d\xi \left[ \cos(\xi \hbar \omega_c/2k_B T_c) \right]. \]  

(14)

Equation (14) immediately gives \(k_B T_c = 0.57 \ h \omega_c \exp(-1/ g(k_F))\). With the aid of data available( for \(g(k_F) = 1.0\) (strong coupling) we have \((\Delta_0/\hbar \omega_c) = 0.5\) from Figure 1, we then obtain the ratio \(2\Delta_0/k_B T_c \approx 4.8\). This value is quite different from the experimental value\[17\] where \(T_c\) is approximately related both to the gap(G) and to the extension of Fermi arcs by \(2G (4\alpha/\pi) = 4.3 \ k_B T_c\) where the angle \(\alpha\) spans the half-Fermi arc as measured from the nodal direction. Though the quantitative aspect of our results may be artefact of the approximations made, qualitatively the exercise underscores the fact that reasonable solution for the order parameter amplitude \(\Delta_0(T=0)\) for an unconventional superconductor is available within the BCS framework.

References

[1] A. Damascelli, Z. Hussain, and Z.-X. Shen, Rev. Mod. Phys. 75, 473 (2003).
[2] P. Kotetes, and G. Varelogiannis, Phys. Rev. B 78, 2205-09 (R) (2008); P. Kotetes, and G. Varelogiannis, Phys. Rev. Lett. 104, 106404 (2010).
[3] C. Zhang, S. Tewari, V.M. Yakovenko, and S. Das Sarma, Phys. Rev. B 78, 174508 (2008); S. Tewari, C. Zhang, V. M. Yakovenko, and S. Das Sarma, Phys. Rev. Lett. 100, 217004 (2008).
[4] M. Franz, Z. Tes’anovic’ and O. Vafek, Phys. Rev. B 66, 054535 (2002).
[5] Y. Wang, L. Li, and N. P. Ong, Phys. Rev. B 73, 024510 (2006).
[6] L. Li, Y. Wang, S. Komiya, S. Ono, Y. Ando, G.D. Gu, and N.P. Ong, Phys. Rev. B 81, 054510 (2010).
[7] A. Kanigel, U. Chatterjee, M. Randeria, M. R. Norman, G. Koren, K. Kadowaki, and J. C. Campuzano, Phys. Rev. Lett. 101, 137002 (2008).
[8] O. Yuli, I. Asulin, Y. Kalcheim, G. Koren, and O. Millo, Phys. Rev. Lett. 103, 197003 (2009).
[9] A. Levchenko, M. R. Norman, and A. A. Varlamov, Phys. Rev. B 83, 020506 (R) (2011).
[10] S. Hufner, M.A. Hossain, A. Damascelli, and G.A. Sawatzky, Rep. Prog. Phys. 71, 062501 (2008).
[11] S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B 63, 94503 (2001); I. Dimov, P. Goswami, Xun Jia, and S. Chakravarty, Phys. Rev. B 78, 134529 (2008); S. Chakravarty, Rep. Prog. Phys. 74, 022501 (2011).
[12] J.-X. Li, C.Q. Wu and D. H. Lee, Phys. Rev. B 74, 184515 (2006).
[13] A. Levchenko, T. Micklitz, M. R. Norman, and I. Paul, Phys. Rev. B 82, 060502(R) (2010).
[14] Jing Xia, Elizabeth Schemm, G. Deutscher, S.A. Kivelson, D.A. Bonn, W.N. Hardy, R. Liang, W. Siemens, G. Koster, M. M. Fejer, and A. Kapitulnik, Phys. Rev. Lett. 100, 127002 (2008).
[15] A. Hackl and M. Vojta, Phys. Rev. B 80, 220514(R) (2009).
[16] The experimental analysis [K. Tanaka, T. Yoshida, A. Fujimori, D.H. Lu, Z.-X. Shen, X.-J. Zhou, H. Eisaki, Z. Hussain, S. Uchida, Y. Aiura, K. Ono, T. Sugaya, T. Mizuno, I. Terasaki, Phys. Rev. B 70, 092503 (2004)] shows that some differences among the different families of cuprate superconductors is strongly correlated with second neighbor hopping.
[17] A. Pushp, C. V. Parker, A. N. Pasupathy, K. K. Gomes, S. Ono, J. Wen, Z. Xu, G. Gu, A. Yazdani, Science 324, 1689 (2009).

**Figure and (figure) caption**

![Diagram](image)

**Figure 1.** The 2-D plot of $(\Delta_0/\hbar\omega_c)$ as a function of the dimensionless coupling strength $g(k_F)$ and second degree polynomial fit.