Studies on Superconducting Pairing Mechanism in Low Dimensional Materials

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By
Soumi Roy Chowdhury

Department of Physics
University of Calcutta

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1) “Investigation of fermionic pairing on tight binding lattice for low dimensional systems – Fermi liquid vs. Luttinger–Tomonaga liquid” **S. R. Chowdhury** and R. Chaudhury Physica B 465 (2015)

2) “Theoretical investigation of the feasibility of electronic mechanism for superconducting pairing in overdoped cuprates with Fermi liquid like and Marginal Fermi liquid- like descriptions for the normal phase” **S. R. Chowdhury** and R. Chaudhury Arxiv:1807.11188v2 (2018) (Communicated to JLTP)

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Chapter 1: Introduction

Understanding superconductivity in low dimensional materials is of paramount importance in view of the discovery of a large number of exotic superconductors in recent times. In my thesis I have considered an electronic excitation based microscopic mechanism to examine the formation of Cooper pairs in a low- dimensional lattice system, in singlet channel with the s-wave like character of the pair wave function. Furthermore, a Fermi sea- like or rather a Fermi liquid- like background has been assumed for the pairing process to take place. Formulation of the problem and application to quasi-1D and quasi- 2D superconductors have been carried out. Though there are other interesting recent discoveries regarding low dimensional superconductors including Fe based superconductors and bisethylenedithio-tetrathiafulvalene for my thesis Tetramethyletetraselenafulvalence salts (TMTSF salts or Bechhgard salts) and overdoped phases of hole- doped cuprates have been chosen [1-6]. In this introduction part the background of my calculation, the history of the earlier works related with this one and the physical properties or characteristics, which my thesis based on are discussed. The second chapter consists of the general pairing equation for the low dimensional systems. The next two chapters are kept for the elaborate pairing scenario in respectively one and two dimensions. Finally there is a section on brief future plan.

Low dimension:

Now what is meant by a low dimensional system? When we are talking about low or reduced dimension we mean that the dimension of the sample is lower than a characteristic length which describe or differentiate the behaviour of electrons from that in higher dimensional systems like mean free path for transport, Fermi wave length for quantization or exciton Bohr radius in semiconductors etc. These characteristics length are bench mark, below this size, if the electrons are confined, then the materials may have new properties than in its bulk form.

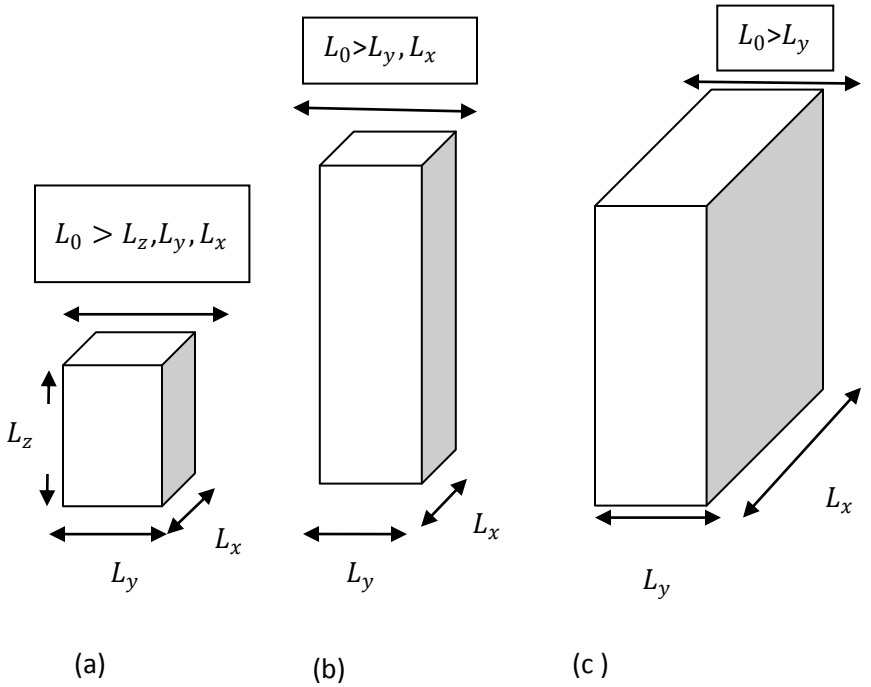

Fig. 1

(a) is three dimensional

(b) is quasi two dimensional

(c) is quasi one dimensional

L_0 here is the characteristic length

These are some of the characteristic lengths, considered frequently:

De Broglie wavelength

Louis de Broglie in 1924 proposed that every kind of particle has both wave and particle properties. Small particles like electron with momentum p, has wavelike properties and the wavelength

associated with it is given by de Broglie wavelength $\lambda = \frac{h}{p} = \frac{h}{m^* v}$ (m* is the effective electron mass). The following figure shows the wave nature associated with electrons in each orbit of an atom

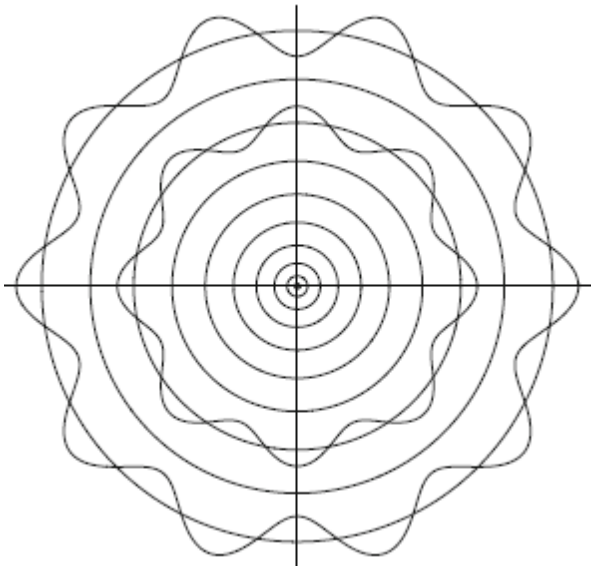

Figure 2: The standing de Broglie wave of electrons in an atom is superimposed on 8th and 10th Bohr radius [7]

The smaller the effective mass the larger is the de Broglie wavelength. Hence new quantum characteristics can be observed if one or two dimensions are of the order of de Broglie wavelength. If the velocity v is given to an electron by accelerating it through a potential difference V, then the work done on the electron is eV. This work done is converted into the kinetic energy of the electron. The expression for de Broglie wavelength is

$$\lambda = \frac{h}{\sqrt{2meV}}$$

This is the wavelength associated with the electron (here relativistic correction of electron mass has been neglected)

We can have a rough idea of the role of de Broglie wavelength on the dimensionality from the theoretical model of Rabinowitz (1993) [8]. As a rough approximation, he considered superconductivity to result simply from a 3D Bose-Einstein (B-E) condensation of the pairs and calculated critical temperatures $T_c = T_c^{BE}$. He shows a comparison of the experimentally observed

transition temperatures, T_c^{Exp} with T_c^{BE} for a series of high-T_c cuprate like compounds, together with the relevant input data for carrier densities, spacings d between adjacent conducting planes, m/m_0=effective/free electron mass, and m_b= 2m**.** The T_c^{BE} are in good agreement with T_c^{Exp} **.** A B-E condensation may occur in 2D-like systems if a small 3D interaction is present [9]. He invoked reduced dimensionality through equipartition principle and a convenient mapping of density of states (g_D) via these following equations

$$g_{3D} = g_3(\epsilon_F) \qquad \text{for 3D system}$$

$$g_{quasi\ 2D} = \frac{g_2(\epsilon_F)}{d} \qquad \text{for cuprates containing array of 2D planes with interplanar spacing d}$$

As

$$n_B = \frac{1}{2}\hbar\omega g_D(\epsilon_F)$$

where n_B is the number density of pairs, ħω is the energy of a Cooper pair [8]

Then

$$n_{quasi-2D} = \frac{(n_B)_2}{d} \qquad \text{for anisotropic 2D material}$$

Where ħω be the energy interval within which incipient bosons (Cooper pairs) are forme, $g_D(\epsilon_F)$ is the density of normal phase electronic states for both spins in D dimensions at the Fermi energy. A B-E condensation occurs when two electron pairs are separated by λ /2 i.e

$$\lambda \approx 2(n_B)^{-1/3}$$

Where λ is de Broglie wavelength [8]. For a pair of electrons of effective mass 2m, momentum p, and kinetic energy $\frac{1}{2}k_BT_c$, the de Broglie wavelength is

$$\lambda = \frac{h}{p} = \frac{h}{[2(2m)\frac{1}{2}k_BT_c]^{1/2}}$$

where f is the number of degrees of freedom per particle pair. For 3D motion of the bosons f = 3. This leads to the B-E condensation temperature in 3D as

$$T_{c3} = \frac{\hbar}{24 k_B m (n_3)^{-2/3}}$$

For anisotropic 2D materials the equipartition of energy principle gives f =2. This yields the transition temperature

$$T_{c2} = \frac{\hbar}{8 k_B m (n_{2/d})^{-2/3}}$$

Rabinowitz then carried out a detailed comparison of the experimentally observed transition temperatures, (T_c^{Exp}) with both calculated T_{c3} and T_{c2} for a series of high-T_c cuprate like compounds using these formulae, with the relevant input data for de Broglie wavelength, carrier densities, spacings d, m/m_0=effective/free electron mass, and m_b= 2m. This investigation shows that T_{c3} rather than T_{c2} are in much better agreement with T_c^{Exp}. We have an important lesson from this result that although formation of pair in cuprates is a 2D phenomenon, transport of pair is completely 3 dimensional [8].

Mean free path:

The mean free path of a particle or molecule is the average distance the particle travels between collisions with other moving particles. $\lambda = (\sqrt{2} n \sigma)^{-1}$, where n is the particle number density and σ is the effective cross sectional area for spherical particles

R. Bardo used the expression of entropy from the scaling theory of Edwards and Thouless and predicted a relationship between mean free path and the dimensionality through his theoretical analysis [10].

$$\lambda_1 = \frac{\pi L}{2} \exp^{\frac{S}{k}} \qquad (1)$$

$$\prod_{k_m} k_m \lambda_2 = \pi \exp^{\frac{S}{k}} \qquad (2)$$

$$\prod_{k_m} k_m \lambda_3 (L_a L_b L_c)^{1/3}) = (3\pi^2/2) \exp^{\frac{S}{k}} \qquad (3)$$

where L is the size of the system, λ is the mean free path between collisions and k_m is the maximum wavevector, S is the entropy regarding any kind of phase transition (whether Pierl's or superconducting type). The ordered electron paired state is reached by minimizing the entropy S in the regime $0 < T \leq T_c$ at a given pressure. From the above equations it is seen that the mean free path determines the behavior of entropy near the second order phase transition for three different dimensional systems. The last two equations can also be applied to quasi 1D and quasi 2D systems respectively. This is when $\lambda_1 \gg \lambda_2$, $\lambda_2 \gg \lambda_3$ so that $S_{quasi1D} \simeq S_{1D}$and $\lambda_2 \gg \lambda_1$, $\lambda_2 \gg \lambda_3$ so that $S_{quasi2D} \simeq S_{2D}$

As the compression stiffens the lattice, dL/dP <0 and according to equation (1) fluctuation decreases. So $dS/dP > 0$. So for superconductivity to occur, critical temperature must decrease with application of pressure (i.e. $dT_c/dP < 0$) which is the case for maximum quasi one dimensional TMTSF salts. For example in case of $(TMTSF)_2PF_6$ dT_c/dP is -0.1K/kbar.

As for the case with the electron-doped high-T_c oxides, S has the 2-D character which will remain unchanged under pressure so that the superconducting transition can occur. In these materials, the interplanar Coulomb repulsion allows the planes to "skate" and retain to their 2D character under pressure. Under these circumstances, $|dT_c/dP| \leq 0.1$K/GPa, since S is independent of L.

TMTSF salts:

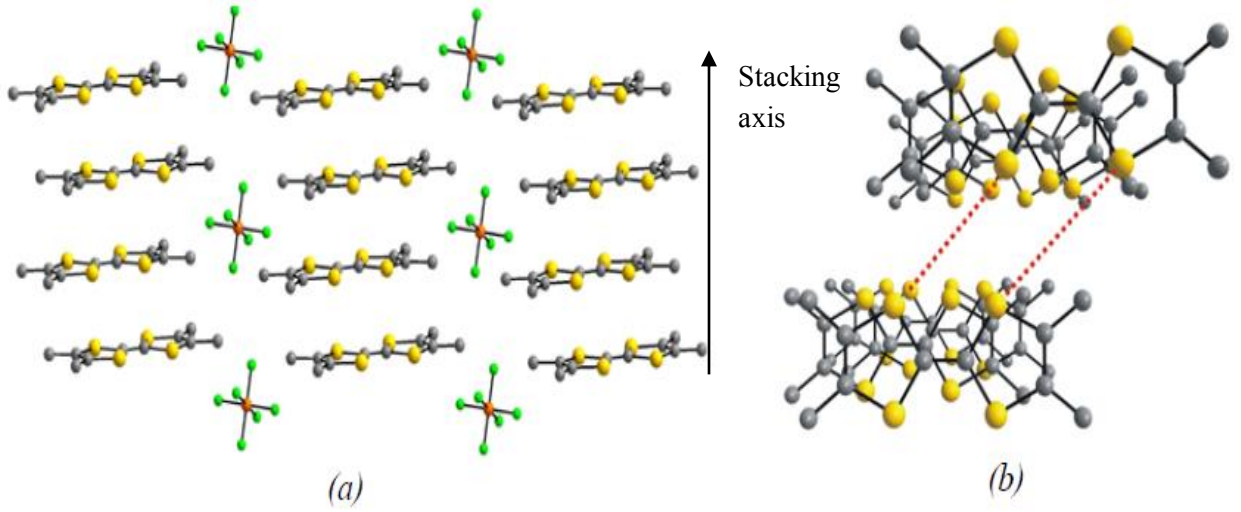

Figure 3: The molecular structure of TMTSF salts [11]

Bechgaard salts with the general formula $(TMTSF)_2X$, where X is a monovalent anion part such as PF_6, ClO_4, AsF_6 etc. was first synthesized by Bechgaard et al. The 2:1 charge transfer salts is formed by transferring one electron from two $TMTSF^+$ ions to one X^- [12]. In most cases the negatively charged anions form a closed shell and do not contribute to the overall conductivity, so current is carried by the holes created on the TMTSF chains and the conductivity depends on the hole density and the complementary mobility. Besides, the size of the anion molecule dictates the spacing of the TMTSF coloumns, and produces an effect similar to that of an applied pressure. In addition to its ionic character, the molecule is also partly covalent. The intramolecular bonding is stronger than the intermolecular effects in this material. Henceforth, the individual molecule approximation mainly decides the character of the bonding. The molecular orbitals from adjacent molecules in the chain overlap constructively resulting in formation of a large bandwidth. This makes the holes delocalized throughout the structure. Besides, a large overlap of electron clouds occurs from the formation of π bonds in between the carbon and selenium atoms of the adjacent TMTSF radicals along the stacking axes (as shown in figure 3a) and perpendicular to molecular plane. In this picture the conductivity takes place in the plane of the paper with vertical direction (stacking axis) The TMTSF family exhibit this crystal structure with stacks of organic molecules separated by the coloumns of negatively charged anions (Figure 3a). The organic molecules are

nearly flat and aligned in a zigzag pattern down along the stacking axis (a direction) with a slight dimerization (figure 3b). The slight overlap between two adjacent stacks in the b direction (in plane and perpendicular to stacking axes) creates a weakly coupled 2-D character as pressure increases. The ratio of electron hopping energy in respectively a, b, and c direction (perpendicular to both plane of the paper and stacking axes) is 0.25:0.025:0.0025, which means electron transfer is 100 times weaker in the weakest axis in comparison with the conducting axis.

Cuprate superconductors:

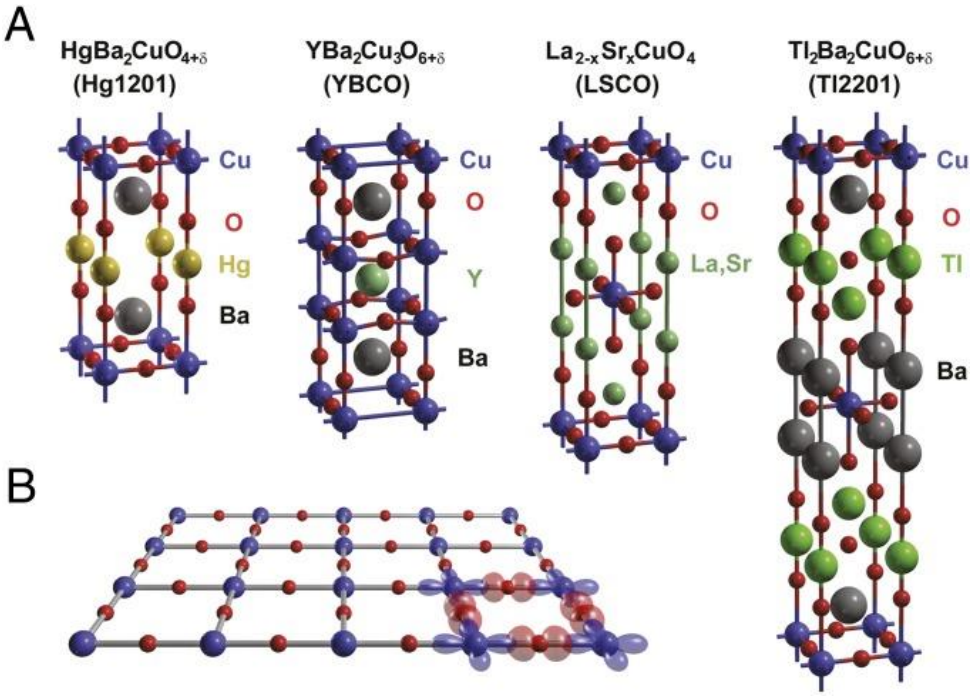

Figure 4: Crystal structures of four cuprates superconductors [13]

The class of cuprates are considered to be quasi-two-dimensional materials with their superconducting properties determined by electrons moving within weakly coupled copper-oxide (CuO_2) layers which form the square lattices of Cu ions coupled with one another through oxygen ions [4,14]. Neighbouring layers containing ions such as lanthanum, barium, strontium, or other atoms act to stabilize the structure and inject electrons or holes onto the copper-oxide layers, resulting in a perovskite structure. The structure of all Cu-oxide superconductors has a block character. Depending on the composition, the elementary cell of a high-temperature superconducting compound can have one, two, and more cuprate layers. In this case, the critical

temperature of the superconducting transition increases with the number of cuprate layers. An elementary cell of La_2CuO_4 is shown here. The maximum $T_c \approx 35$ K. The size of the cell is characterized by the following parameters: a = b = 3.77 Å, c = 13.25 Å. Thus, the high-temperature superconductors are characterized by both large volumes of elementary cells and a clearly manifested anisotropy of layers.

The following discussions are on the few additional important aspects related to superconductors in general including the low dimensional ones.

1) Fermi liquid (FL) Theory (For normal phase):

L. Landau put forward an idea that a weakly interacting 3- dimensional Fermi system is composed of some effective particles (quasi-particles) that behave as almost free fermions excepting that their masses and other characteristics are different from the corresponding non-interacting values [15]. If we promote only one particle to a state above the Fermi surface, the interaction will change the energy of all other fermions. However, Landau assumed that weakly excited states with energies near the Fermi level, can be described as a superposition of elementary excitations (quasi-particles) which behave almost as free particles, with an effective mass m* different from the bare mass m, although the original system may as well be a highly interacting one i.e.

$$\delta E[\delta n] = \sum_{\vec{p},\sigma} \varepsilon_p \delta n(\vec{p}) + \sum_{\vec{p},\vec{p'}} \sum_{\sigma,\sigma'} f_{\sigma,\sigma'}\left(\vec{p},\vec{p'}\right) \delta n_\sigma(\vec{p}) \delta n_{\sigma'}(\vec{p'})$$

Where δn is the number of quasi particles producing excitation energy δE and the higher order correction describes the interaction among quasi particles with $f_{\sigma,\sigma'}(\vec{p},\vec{p'})$ denoting interaction strength. If the system is isotropic and there is no magnetic field present, the quasiparticle with up spin (↑) has the same energy as the quasiparticle with down spin (↓). Likewise, the interaction between quasiparticles depends only on the relative orientation of the spins σ and σ'. So $f_{\sigma,\sigma'}(\vec{p},\vec{p'})$ can be expressed by two additive parts viz. one is symmetric and corresponds to charge and the other is antisymmetric and corresponding to spin. The spin symmetric interaction is related proportionaly to the effective mass. The density- density correlation function in Fermi liquid is defined as

$$\rho(r - r') = (1/\Omega) \sum_{k'<k_F} e^{ik'.(r-r')\}} = \frac{{k_F}^3}{2\pi^2} \{ \frac{Sin(k_F|r - r'|)}{(k_F|r - r'|)^3} - \frac{Cos(k_F|r - r'|)}{(k_F|r - r'|)^3} \}$$

Where Ω is the normalization constant having dimensions of volume and k_F is the Fermi momentum. The expression shows how the electrons are distributed at r'around r.

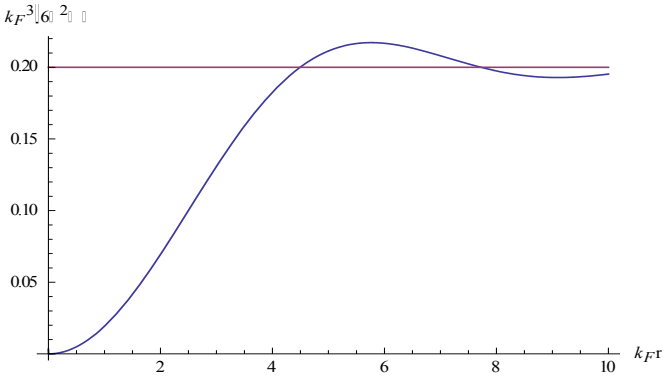

Figure 5- Distribution of electrons with spin parallel to that of the electron situated at r=0

Adding the effect of electron electron interaction changes the energy of a single particle near the Fermi energy and is represented by Fermi liquid theory. To consider the e-e interaction effect, for high density electron gas the Hartree- Fock approximation and correlation corrections are generally adopted. There is however no satisfactory treatment even now of the influence of e-e interaction on quasi particle properties for general electron density. A rough resemblance of lattice effect can be mapped on this model by introducing a band structure effective mass $\tilde{m}$ instead of bare electron mass m. Kohn- Luttinger demonstrated a method of deriving $\tilde{m}$ using k.P perturbation theory [16]. So we can think of an almost Fermi liquid like picture with effective mass $\tilde{m}^*$ to describe interacting fermions on lattice in the high fermionic density limit, as is often encountered in real condensed matter systems. The simple Fermi liquid theory breaks down in the following cases: 1) Two-channel Kondo models- when two independent electrons can scatter from a magnetic impurity it leaves behind 'half an electron' [17]. 2) Disordered Kondo models. Here the scattering from disordered magnetic impurities is too strong to allow the Fermionic quasiparticles to form [18]. 3) Underdoped Mott- Hubbard insulators or very low density electron gas leading to Wigner solid [19]

2) s- wave, p- wave and d- wave superconducting pairing:

A superconducting (Cooper pair) wavefunction has both a spin and an orbital (spatial) component. An s-wave and d- wave superconductor corresponds to a singlet state with {S=0; angular momentum ℓ=0} and {S=0; ℓ=2} respectively while the p-wave refers to a triplet state with {S=1; ℓ=1} [11]. The non-spin part of the superconducting order parameter can be expressed as $\Psi(\vec{k}) \approx \Delta(\vec{k})e^{ik\varphi(\vec{k})}$, where $\Delta(\vec{k})$ is the magnitude of the superconducting gap and $\varphi(\vec{k})$ is the phase of the order parameter, both of which may have a momentum-dependence in k-space [20]. The magnitude of a superconducting gap roughly represents the energy required to break a Cooper pair. The phase is a factor that the superconducting wavefunction aquires spontaneously below the transition temperature (Tc). In momentum space, a s-wave superconducting gap has isotropic magnitude in all directions, and it has a fixed phase in all directions.

Examples of the systems where different types of pairings are seen:-

s-wave: Elemental superconductors such as Al, Nb, and Pb and binary like $MgBr_2$, Y_9Co_7, high T_C cuprate superconductors and Fe- pnictides [21]

d-wave: Cuprate high temperature superconductors, Heavy Fermion superconductors, Fe- pnictides [21]

p- wave: Sr_2RuO_4[22]

The above systems include both FL- characterized normal phases as well as those with non- Fermi liquid ones.

3) Excitonic Mechanism:

An exciton denotes a system of an electron and a hole bound together by their Coulomb interaction. When a photon excites an electron into the conduction band, a hole is left behind in the valence band; the electron, having a negative charge will be attracted to this hole and may (provided the energy is not too large) bind to the positively charged hole forming an exciton. Thus, the excitonic state is a bound state and represents a lower energy state than the band states. Therer are mainly three kinds of exciton as discussed below:-

1) In materials with a small dielectric constant, the Coulomb interaction between an electron and a hole is strong and so the exciton tends to be small, of the same order as the size of the unit cell and

is entirely located on the same molecule, as in fullerenes [23]. This is Frenkel exciton with a typical binding energy of the order of 0.1 to 1 eV. Frenkel excitons are typically found in alkali halide crystals and in organic molecular crystals composed of aromatic molecules, such as anthracene and tetracene [24].

2) Wannier exciton states in 3D semiconductors are generally observed in very pure samples and at very low temperatures. In semiconductors, the dielectric constant is generally large. Consequently, electric field screening tends to reduce the Coulomb interaction between electrons and holes [25]. The binding energy is usually much less than that of a hydrogen atom, typically of the order of 0.01eV. The criterion for the stability of the Wannier exciton is that the average Bohr orbit of the exciton should be less than the distance between impurities. Let a very pure sample (10^{14} impurities/cm^3) is doped lightly (to 10^{16} impurities/cm^3). A carrier concentration of 10^{16}/cm^3 corresponds to finding an impurity ion within every 100 Å from some lattice point. The excitonic spectrum would be attenuated because of screening effects associated with the charged impurities. Let us consider an excitonic radius of around 100Å. If an impurity ion is located within this effective Bohr radius, then the electron- hole Coulomb interaction is screened by the impurity ion and the sharp spectrum associated with the excitons will disappear. Also in case of exciton in the indirect gap semiconductor because of the large difference in crystal momentum $\hbar k$ between the valence band extremum and the lowest conduction band minimum, the exciton may acquire a large center of mass momentum corresponding to the momentum of the absorbed or emitted phonon $\hbar q$. For the indirect exciton, a large range of crystal momentum $\hbar k$ values are possible and hence the exciton levels spread out into bands.

3) In between the above two varities there exists another kind of exciton called charge transfer (CT) exciton. This is defined as a crystal state in which a hole and an electron, mainly on the adjacent sites, are bound together by their Coulomb force and diffuse as a pair within a near neighbour location [26]. The energy required to produce the CT exciton, must be less than that required to ionize a molecule completely.

The first attempt to explore occurrence of superconductivity by invoking exciton was made by W. A. Little in 1964 [27]. He created a model consisting of two parts, a long chain called the "spine" in which electrons fill the various states and secondly, a series of arms or side chains attached to the spine as indicated in the following figure. He has shown that by appropriate choice of the molecules

which constitute the side chains, the oscillation of charge in these side chains can provide an interaction between the electrons moving in the spine. Let an electron in the spine near point P is in stable equilibrium with the electrons in the adjacent side chain of B. If the oscillating electron in the side chain goes further from the spine then the next electron in the spine becomes a bit loosely bound and feels attracted towards the previous electron in the spine.

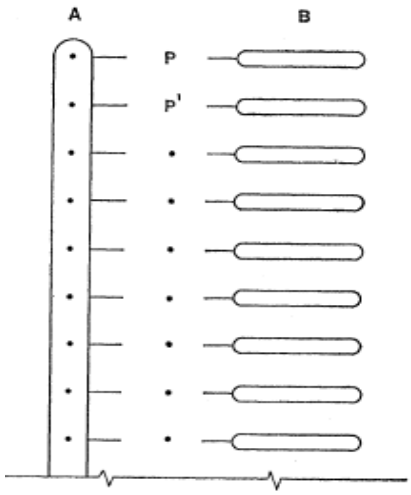

Figure 6: Proposed model of a superconducting organic molecule. The molecule A is a long unsaturated polyene chain called the spine. The molecules B are side chains attached to the spine at points $\mathbf{P}, \mathbf{P}'$….[27]

An assumption has been made here that in this model there is negligible overlap between side chains, and also overlap between sites on the spine is relatively small. Though there is a very weak coupling between the stacks of $(TMTSF)_2X$ as is here in between the side chains of this model, no successful attempt of the incorporation of this theory on $(TMTSF)_2X$ has been made yet. Also the electronic transport in this model was not considered to be taken place in the way it happens in TMTSF salts through overlapping of π bonds (Reference: Introduction- Subtopic: TMTSF salts)

The possibility of the existence of two-dimensional superconductors was first proposed in 1964, much before the discovery of quasi two dimensional high- Tc superconductors [28]. The proposed mechanism was exciton based mechanism where the phonons are replaced by electronic excitations in a system of bound electrons. The excitonic energy range $\hbar\omega_{ex} = k_B\theta_{ex}$ was taken to be of the order of 0.1-1 eV corresponding to the temperature $\theta_{ex} \sim 10^3 - 10^4$K. Substituting this value in

place of θ_{phonon} in the BCS formula

$$T_C = \theta_{ex} \exp(-\frac{1}{\lambda})$$

(Where λ is the coupling constant) the critical temperature was obtained as high as 500K.
They say that `paper will withstand anything', but realization of such possibilities hasn't taken place till date.

In 1966 Toyazawa et al formed a model of an excited system with a hole in the valance band, attracting the electron in the conduction band through the square well potential extending over 3 atoms, with the hole in the central atom. There is an interaction V between electrons of neighbouring atoms [29]. The atomic site energy difference is Δ and the tight binding transfer integral is t. When the potential depth V is comparable to the half band width 2t (the model for ionic crystal), one can observe both local structure and band structure in the continuous spectrum. Varma adopted this model and incorporated it for the Cu and O atoms of the CuO_2 plane of the doped La_2CuO_4. The relevant 2t to compare with V for strong localized excitonic effects then is the hopping amplitude connecting anti bonding and bonding orbitals [30].

In tetragonal La_2CuO_4, band structure calculations show that the copper $d_{x^2-y^2}$ orbitals hybridize with the oxygen p_x and p_y orbitals leading to a bonding band about 2.5 eV wide and an anti-bonding band separated by about 3.5 eV which is about 3.5 eV wide. For undistorted La_2CuO_4, the anti-bonding band is half-full. The one electron in this band is shared by the copper and the two oxygen atoms per unit cell in the basal plane. This implies that Cu fluctuates between Cu^{++} and Cu^{+} states while the two oxygen atoms fluctuate between O^{--} $O^{--}$and O^{--} O^{-} states. In the acceptor-doped superconducting materials, the hole density is quite low ($\leq 10^{22} cm^{-3}$). This gives an interparticle spacing $r_s \geq 3$ Å which is larger than the Cu-O separation of 1.9 Å in the basal plane. Thus we expect the charge transfer excitation $Cu^{++}O^{--} \rightarrow Cu^{+}O^{-}$ to be essentially unscreened. The unscreened energy difference or the difference in kinetic energy between these two configurations in a tight binding basis set within the unit cell is equal to the difference between the average bonding and antibonding band energy, which is about 6 ev. This indicates the possibility of a well localized unscreened particle-hole excitation (charge transfer exciton) of some energyω_0. Based on this model, Varma estimated the value of ω_0 to be ~0.5 eV for Lanthanum based cuprate superconductors [30].

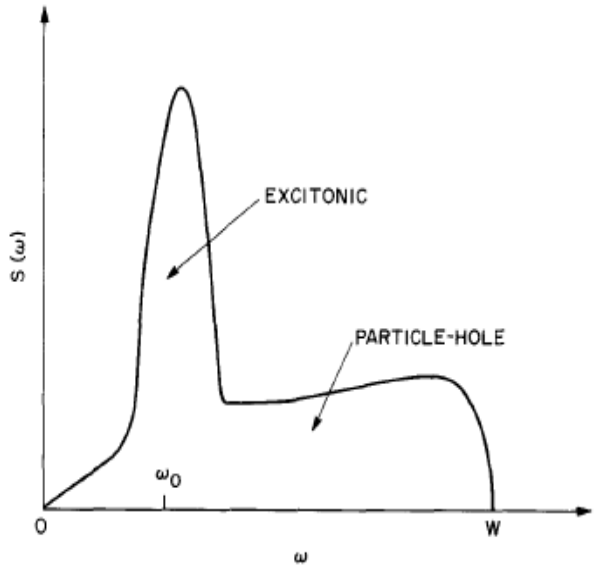

Figure 7: Schematic spectral weight of $\mathbf{La_2CuO_4}$. The particle hole spectrum extends to the bandwidth W and the charge transfer excitonic feature occurs around $\boldsymbol{\omega_0}$ [30]

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2. General Equation for Pairing Instability

An electron pair in a superconductor does not behave like a point particle but instead its influence extends over a distance of about 1000 Å depending on value of coherence length of different superconductors. But there are many other Cooper pairs in this region and the spheres of influence of the pairs overlap extensively. These electrons continually exchange partners with each other i.e. they interact with each other. Overlap between the waves of the two electrons in a pair and then between the waves associated with the pairs results in the coherence or long range order which in turn can sustain persistent current in superconducting material.

But in a purely low dimensional material supercurrents cannot persist for a long time and must decay mainly because of the absence of the phase transitions in low dimensional systems i.e. the absence of a long range order at finite temperature.

The absence of long-range order of this simple form has been shown by Mermin and Wagner (1968) using rigorous calculation [1]. The Mermin–Wagner theorem states that continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $d \leq 2$. The theorem can be conceptualized for low dimension that the excitation of spinwaves can destroy the ferromagnetic order [2].

Let the temperature-dependent magnetisation is$M(T) = M(T = 0) - \Delta M(T)$, where $\Delta M(T)$ is the reduction of the magnetisation due to thermally excited spin-waves. $\Delta M(T)$ is calculated integrating over the density of states (DOS) N(E) of the excitations times their the probability for the thermal occupation

$$\Delta M(T) \sim \int_0^{\infty} N(E)\left[\frac{dE}{e^{\frac{E}{k_B T}}-1}\right]$$

DOS depends on the dimensionality of the system. The general case of excitations with a dispersion

$$E \sim k^n$$

is having a volume element in d-dimensional k space

$$dv = k^{d-1}dk$$

So

$$E^{\frac{d-1}{n}} \sim k^{d-1}$$

Hence the DOS is

$$N(E) \sim E^{\frac{d-n}{n}}$$

Therefore for n=2 (dispersion of spin waves in ferromagnetic with Heisenberg- Hamiltonian model) and d=2 (two dimension) we have constant DOS and

$$\Delta M(T) \sim \int_0^{\infty} \text{constant} \left[\frac{dE}{e^{\frac{E}{k_B T}} - 1}\right]$$

$$\sim T \int_0^{\infty} \left[\frac{dE}{e^{\frac{E}{k_B T}} - 1}\right]$$

For small $\frac{E}{k_B T}$,

$$e^{\frac{E}{k_B T}} - 1 = \frac{E}{k_B T}$$

So we find that

$$\Delta M(T) \sim \int_0^{\infty} \left[\frac{dE}{\frac{E}{k_B T}}\right]$$

diverges logarithmically. This means that ΔM(T) diverges for finite T, indicating the breakdown of magnetic order for T > 0.

The reason for the absence of this order was also suggested by Peierls (1935) [3]. He has argued that thermal motion of long-wavelength phonons will destroy the long-range order of a two-dimensional solid in the sense that the mean square deviation of an atom from its equilibrium position increases logarithmically with the size of the system.

Anderson has created a model relating ferromagnetism to superconductivity and using this one can show that the theory of the absence of long range order in the low dimensional ferromagnetic material holds in low dimensional superconducting material too at finite temperature [4].

Anderson observed that if one considers a Cooper pair state to be identified with a “down-spin state” and the absence of a pair to be represented by a “up spin state” in particle hole space, i.e.

no pair: $|\Uparrow\rangle \equiv |0\rangle$,

pair: $|\Downarrow\rangle \equiv c^{\dagger}_{k\uparrow}c^{\dagger}_{-k\downarrow}|0\rangle$

then the BCS ground-state is revealed as a kind of Bloch domain wall formed around the Fermi surface. The BCS theory involves three key operators viz. the number operator $n_{k\uparrow} + n_{-k\downarrow}$, the pair creation and pair annihilation operators, $b^{\dagger}_{k} = c^{\dagger}_{k\uparrow}c^{\dagger}_{-k\downarrow}$ and $b_k = c_{-k\downarrow}c_{k\uparrow}$ respectively. Here these operators are further introduced as the components of a pseudo-spin. In the subspace where $n_{k\uparrow} + n_{-k\downarrow}$is either 0 or 2, the pseudospin takes the form

$$2s_z = 1 - n_k - n_{-k} = \begin{matrix} \\ \text{empty} \\ \text{full} \end{matrix} \begin{matrix} \begin{matrix} \text{empty} & \text{full} \end{matrix} \\ \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \end{matrix}$$

so that a fully occupied k state is a "down" pseudo-spin state, and an empty k-state is an "up" pseudo spin state. Similarly, the raising and lowering operators represent respectively, the pair destruction and creation operators, viz.

$$b_k = s_{xk} + is_{yk} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad b^{\dagger}_{k} = s_{xk} - is_{yk} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Thus in this description, the BCS reduced Hamiltonian given by

$$H_{RED} = -2\sum_{k} \epsilon_k s_{zk} - \sum_{k,k'} V_{k,k'}\,(s_{xk} + is_{yk})(s_{xk'} - is_{yk'})$$

is a kind of anisotropic quantam spin model defined in momentum space. Anderson showed that in this language, the metal is a sharp domain wall along the Fermi surface while the superconductor has a soft "Bloch domain wall" (Fig 2a) in which the pseudospins rotate continuously from down (full) to sideways (linear combination of full and empty) to up (empty).

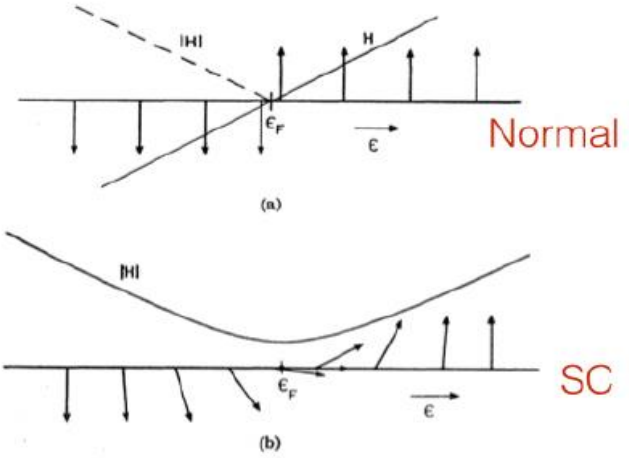

Figure 2: a) In Anderson domain wall interpretation of superconductivity the normal Fermi liquid is a sharp domain wall where the weiss field H vanishes at the Fermi surface. b) In the superconductor the pseudospins rotate smoothly and Weiss field never vanishes, giving rise to a finite gap [4].

The previous analysis establishes that long range superconductivity can't occur in pure 1 or 2-dimensional systems at finite temperature, however the formation of cooper pair at very low temperature can still take place there. Besides, the word 'quasi' is very significant while discussing pure 1 or 2- dimensional systems. I had stated earlier in the introduction part that the materials I am working with are quasi 1- dimensional and quasi 2- dimensional systems. I now clarify that my treatment involving pairing theory is based on the following hypothesis:- the phenomenon of superconductivity in quasi one dimensional and quasi two dimensional systems arises predominantly as a combination of two distinct processes viz.

1) Cooper pair formation in a preferred chain/ layer i.e. intra- chain/ intra layer pair formation accompanied by

2) inter- chain/ inter- layer pair tunneling at very low temperatures.

The above hypothesis can be considered as the building block for the construction of microscopic theory for superconductivity in these low- dimensional anisotropic systems.

In quasi- one dimensional organic superconductor $(TMTSF)_2X$, $t_\perp$ (the interchain single electron tunneling parameter) is an increasing function of induced pressure and this has a direct connection with the critical temperature T_c. A lot of work has been done on a system consisting of an infinite array of parallel metallic chains linked by a coupling parameter $t_\perp$. It was found that, as $t_\perp$ is increased from zero, but much less than Δ, where Δ is the superconducting gap energy corresponding to the 1D system, then T_c increases with increasing $t_\perp$. But when $t_\perp > \Delta$, then T_c has a reciprocal relation with $t_\perp$. (Though out of context here but it is interesting to note that Δ gets related to T_c here like the well known BCS equation). It results from loss of coherence as hopping between chains takes place via individual electrons at large $t_\perp$ instead of electron pairs at low $t_\perp$. Therefore, for a lower magnitude of $t_\perp$ (or by applying a lower amount of pressure) an enhancement in T_c can be achieved as pair tunneling becomes more favourable than individual carrier hopping in this regime.

By studying the spectral density of the single particle excitations in quasi- two dimensional high temperature cuprate superconductors, Chakravarty and others have built a formalism, in which the Josephson critical current I_c is proportional Δ^2/ω_c, where Δ is the superconducting gap and ω_c is the frequency scale of the order of the in-plane bandwidth [6]. In contrast, for a superconductor with Fermi liquid characterized normal phase, this is not possible because I_c is proportional to$|\Delta|$. The restructuring of the Josephson- effect allows one to form an interlayer Tunneling Hamiltonian in a non Fermi liquid background at sufficiently low energies and low temperatures in underdoped and optimally doped cuprate superconductors [6]. This implies emergence of superconductivity due to pair hopping through copper- oxide planes in HTSC, unlike single particle tunneling between the layers. This prominent class of examples of the exception from Fermi liquid theory refer to the metallic state above the superconducting transition temperature Tc near optimal doping. The strange metal phase exhibits thermodynamic and transport behavior significantly different from those of an ordinary metal. A particularly striking property of this metal phase is that the electrical resistivity increases linearly with temperature, in contrast to the quadratic temperature dependence of an ordinary metal. This remarkably simple behaviour is existing over a wide range of temperature, appearing in all cuprate superconductors. The anomalous behaviour can be answered with the help of photoemission experiments which can probe directly a Fermi surface and its low energy

excitations. In an Angular Resolved Photoemission Spectropy (ARPES) experiment, incident photons knock out electrons from the sample and the intensity $I(k, \omega)$ of the electron beam is proportional to$A(k, \omega)f(\omega_k)$, where $f(\omega_k)$ is the Fermi-Dirac distribution and $A(k, \omega)$ is the electron spectral function defined by

$$A(k, \omega) = -(\frac{1}{\pi}) \text{ Im } G(k, \omega)$$

ARPES experiments indicate that a Fermi surface still exists, but excitations exhibit a much broader peak than that for a Fermi liquid. The experimental results can be fit well to the following expression, postulated as "Marginal Fermi liquid" (MFL) [7],

$$G(k, \omega) = h/(\omega - v_F(k - k_F) + \Sigma(k, \omega))$$

with the self-energy $\sum(\omega, T)$ of the electrons behaves like $\sum^{Re}(\omega, T) \sim \omega \ln|\omega|$ and $\sum^{Im} \sim |\omega|$ for $\omega > T$ in contrast to ordinary Fermi liquid theory where $\sum^{Re}(\omega, T) \sim \omega$ and $\sum^{Im} \sim \omega^2$

Let us start by recalling the story for a non-interacting Fermi gas (e.g. a gas of electrons in a box) for which the many-particle states can be obtained by simply filing single-particle energy eigenstates following the Pauli exclusion principle. The ground state is then given by filling all the (single-particle) states inside a sphere in momentum space with radius k_F determined by the density of fermions and with all states outside the sphere empty. The locus of points in momentum space at the boundary of this sphere, $k \equiv |k| = k_F$, is called the Fermi surface. The low-energy excitations of the system are given by either filling a state slightly outside the Fermi surface or removing a fermion from a filled state slightly inside the Fermi surface, and are called a particle and hole respectively. These excitations are gapless and have a linear dispersion ($(k - k_F) \ll k_F$):

$$\epsilon_F = \frac{k^2}{2m} - \frac{{k_F}^2}{2m} = \frac{1}{2m}(k + k_F)(k - k_F) \equiv \frac{2k_F}{2m}(k - k_F) = v_F(k - k_F)$$

Particles and holes are distinguished by the sign of $(k - k_F)$. At a field theoretical level, these excitations manifest themselves as poles in the complex frequency plane of the retarded Green's function $G(k, \omega)$ for the electron operator in momentum space

$$G(k,\omega) = \frac{1}{\omega - \epsilon_k + i0_+}$$

where ω is quasiparticle energy. The propagation of a particle of energy can be obtained by fouruer transforming this.

$$G(t,k) = \theta(t)e^{i\epsilon_k t}$$

The situation becomes complicated once we switch on interactions between fermions. An electron travelling in a solid distorts the lattice because of the Coulomb interaction with the ions. The lattice distortion in turn has a feedback on the electron dynamics, resulting in an increase of the electron mass and a shortening of the electron lifetime in a particular quasi-particle state. Within quantum field theory, this effect is described in terms of a complex self-energy $\sum^{Im}$ that the electron acquires. The real part of the self-energy describes the change in the electron energy, and the imaginary part provides information on the electron lifetime τ or scattering rate $1/\tau$ through $\tau = \hbar/\sum^{Im}$

Landau's Fermi liquid theory postulates that the qualitative picture for a non-interacting gas persists for generic interacting fermionic systems [8]. In particular, it assumes that despite strong interactions among fundamental fermions, the low energy excitations near the Fermi surface nevertheless behave like weakly interacting particles and holes, which are called quasi-particles and quasi-holes. They have the same electrical charge as those of fundamental fermions and obey Fermi statistics. The dispersion of a quasi-particle (similarly for a quasi-hole) resembles in free theory

$$\epsilon(k) = v_F(k - k_F)$$

$$v_F = k_F/m^*$$

where $m*$ can be considered as the effective mass of the quasi-particle and is in general different from the original fermion mass m, from renormalization by many-body interactions. When turning on interactions, a particle (or hole) can now decay into another particle plus a number of particle-hole pairs. But it is not difficult to check that the exclusion principle constrains the phase space around a Fermi surface so much, that given generic local interactions among particles and holes, the decay (or scattering) rate of a particle (or hole) obeys

$$\tau \sim \epsilon^2(k)$$

where ϵ is the energy of a particle (or hole). Thus, despite potentially strong interactions, particle or hole excitations near the Fermi surface have a long lifetime still applies. Thus for a Fermi liquid, the fourier transformed Green's function should be modified to

$$G(t,k) = \theta(t)e^{i(\epsilon_k t - \frac{\tau}{2}t)}$$

which implies that near the Fermi surface the retarded function for the electron operator should have the form

$$G(k,\omega) = \frac{Z}{\omega - v_F(k-k_F) + \Sigma(k,\omega)}$$

with the self-energy $\Sigma(\omega, k)$

$$\Sigma = \frac{i\tau}{2} \sim i\omega^2$$

The residue $Z \leq 1$ of the pole, which is called the quasiparticle weight, can be interpreted as the overlap between the (approximate) one-quasiparticle state with the state generated by acting the electron operator on the vacuum. It is essentially the weightage of the coherent part of the propagator.

But with the self-energy $\sum(k,\omega)$ given by $\sum(k,\omega) \approx C\omega\ln|\omega| + D|\omega|$,where C real and D complex, we see that the system appears to possess gapless excitations of dispersion relation $= v_F(k-k_F)$. However, the decay rate τ of such excitations, which is given by the imaginary part of Σ, is now proportional to ω in contrast to ω^2 for a Fermi liquid. The decay rate, which is comparable to ω, is so large, that an excitation will already have decayed before it can propagate far enough (i.e. one wavelength) to show its particle-like properties. As a result, such an excitation can no longer be treated as a quasiparticle. Also the residue for the pole in the complex plane scales like $Z \sim 1/\ln(k-k_F)$ as the Fermi surface is approached and thus the quasiparticle weight vanishes logarithmically. Thus at the Fermi surface the overlap of an excitation with original electrons vanishes. Mathematically, the singularity of $A(k,\omega)$ at $k = k_F$ and $\omega = 0$ is much softer than that for a Fermi liquid. Thus the strange metal phase of cuprates has a Fermi surface (i.e. there still exist a surface in momentum space which has gapless

excitations), but the quasiparticle picture breaks down. From the perspective of renormalization group, it must be that the system is flowing to a nontrivial fixed point distinct from that for a Fermi liquid.

Before I discuss my pairing investigation on low dimensional lattices it would be helpful to briefly review the conventional Cooper's one pair problem in continuum [9].

In the presence of an attractive interaction, the free electron state becomes unstable. The instability can be understood by considering two particular electrons of coordinates $\overrightarrow{r_1}$ and $\overrightarrow{r_2}$, The other electrons are still being treated as a free electron gas. Let $\psi(\overrightarrow{r_1}, \overrightarrow{\sigma_1}, \overrightarrow{r_2}, \overrightarrow{\sigma_2})$ be the wavefunction of the two electrons. Then

$$\psi(\overrightarrow{r_1}, \overrightarrow{\sigma_1}, \overrightarrow{r_2}, \overrightarrow{\sigma_2}) = \varphi_{\vec{k}}(\overrightarrow{r_1}) e^{i\vec{K}.\vec{R}} \chi(\overrightarrow{\sigma_1}, \overrightarrow{\sigma_2}) \qquad (1)$$

Where $\vec{R}$ is the centre of mass $\vec{R} = \frac{\overrightarrow{r_1}+\overrightarrow{r_2}}{2}$, $\vec{r} = \overrightarrow{r_1} - \overrightarrow{r_2}$ and $\overrightarrow{\sigma_2}$ and $\overrightarrow{\sigma_2}$ denote the spins of the electrons (up or down) and (↑ or ↓)and $\hbar\vec{k}$ is the centre of mass momentum; $\varphi_{\vec{k}}(\vec{r})$ is the wavefunction in the relative co- ordinate space and χ denotes the spin wavefunction (spin orbit coupling is neglected). In what follows we assume that pairing takes place in a singlet state for which

$$\chi = \frac{1}{\sqrt{2}}\left[\binom{1}{0}\binom{0}{1} - \binom{0}{1}\binom{1}{0}\right].$$

Since the system is assumed to be translationally invariant and one neglects spin- dependent forces, the centre of mass $\hbar\vec{k}$ of the pair and the total spin S are constants of motion. The orbital wave function of the pair can be written as,

$$\psi(\overrightarrow{r_1}, \overrightarrow{r_2}) = \varphi_{\vec{K}}(\vec{r}) e^{i\vec{K}.\vec{R}}$$

Where ;

$$\varphi_{\vec{K}}(\vec{r}) = \sum_{\vec{k}} a_{\vec{k}}\, e^{i\vec{k}.\vec{r}}$$

(the basis wave functions are assumed to be plane wave functions in the case of continuum and if the wavevector of one electron is $\vec{k} + \frac{\vec{K}}{2}$ and the another one $-\vec{k} + \frac{\vec{K}}{2}$. So,

$$\psi(\vec{r_1},\vec{r_2}) \equiv \varphi_{\vec{K}}(\vec{r}) = \sum_{\vec{k}} a_{\vec{k}}\, e^{i\vec{k}.\vec{r}} e^{i\vec{K}.\vec{R}} = \sum_{\vec{k}} a_{\vec{k}}\, e^{i(\vec{k}+\frac{\vec{K}}{2}).\vec{r_1}}\, e^{-i(\vec{k}-\frac{\vec{K}}{2}).\vec{r_2}} \qquad (2)$$

For zero centre of mass momentum $|\vec{K}| = 0$. So equation (2) reduces to

$$\psi(\vec{r_1},\vec{r_2}) \equiv \varphi_{\vec{K}}(\vec{r}) = \sum_{\vec{k}} a_{\vec{k}}\, e^{i\vec{k}.\vec{r}} = \sum_{\vec{k}} a_{\vec{k}}\, e^{i\vec{k}.\vec{r_1}}\, e^{-i\vec{k}.\vec{r_2}}$$

The terms $e^{i\vec{k}.\vec{r_1}}$ and $e^{-i\vec{k}.\vec{r_2}}$ can be thought of as single particle states of momentum $\vec{k}$ and $-\vec{k}$, we see that the pair wave function is a superposition of configuration in each of which a definite pair state $(\vec{k},-\vec{k})$ is occupied. Here $a_{\vec{k}}$ is the probability amplitude for finding one electron in the plane- wave state of momentum $\hbar\vec{k}$ and the other electron in the state $-\hbar\vec{k}$

Now from the Schroedinger equation for the two electrons is

$$-\frac{\hbar^2}{2m}\left(\nabla_1{}^2 + \nabla_2{}^2\right)\varphi(\vec{r}_1-\vec{r}_2) + V(\vec{r}_1,\vec{r}_2)\varphi(\vec{r}_1-\vec{r}_2) = \epsilon\varphi(\vec{r}_1-\vec{r}_2) \qquad (3)$$

Where ϵ is the energy eigen value of the pair, Now we proceed further by multiplying with $\varphi^*(\vec{r}_1-\vec{r}_2)$ the both sides of the above equation, using the form of $\varphi(\vec{r})$

$$\sum_{\vec{k},\vec{k'}} \frac{\hbar^2}{2m}\left[\left(\vec{k}+\vec{K}/2\right)^2 + \left(\vec{k}-\vec{K}/2\right)^2 a_{\vec{k}} a_{\vec{k'}} \int d^3r_1 e^{i\left(\vec{k}-\vec{k'}\right).\vec{r_1}} \int d^3r_2 e^{i\left(\vec{k}-\vec{k'}\right).\vec{r_2}}\right.$$

$$+ \sum_{\vec{k},\vec{k'}} a_{\vec{k}} a_{\vec{k'}} \iint d^3r_1 d^3r_2 e^{i\vec{k}.\vec{r_1}} e^{-i\vec{k'}.\vec{r_1}} V(\vec{r}_1,\vec{r}_2) e^{i\vec{k'}.\vec{r_2}} e^{-i\vec{k}.\vec{r_2}}$$

$$= \sum_{\vec{k},\vec{k'}} \epsilon a_{\vec{k}} a_{\vec{k'}} \int d^3r_1 e^{i\left(\vec{k}-\vec{k'}\right).\vec{r_1}} \int d^3r_2 e^{-i\left(\vec{k}-\vec{k'}\right).\vec{r_2}}$$

$$\sum_{\vec{k},\vec{k'}} \frac{\hbar^2}{2m}\left[\left(\vec{k}+\vec{K}/2\right)^2 + \left(\vec{k}-\vec{K}/2\right)^2 a_{\vec{k}} a_{\vec{k'}}\, \delta^2{}_{\vec{k},\vec{k'}} + \sum_{\vec{k},\vec{k'}} a_{\vec{k}} a_{\vec{k'}} V_{\vec{k},\vec{k'}} = \sum_{\vec{k},\vec{k'}} \epsilon a_k a'_k \delta^2{}_{\vec{k},\vec{k'}}\right.$$

$$a_{\vec{k}} \frac{\hbar^2}{2m}\left[\left(\vec{k}+\frac{\vec{K}}{2}\right)^2 + \left(\vec{k}-\frac{\vec{K}}{2}\right)^2\right] + \sum_{\vec{k'}} a_{\vec{k'}}\, V_{\vec{k},\vec{k'}} = \epsilon a_{\vec{k}} \qquad (4)$$

The quantity $V_{\vec{k},\vec{k'}}$ is the Fourier transform of the attractive contact interaction $\left(-u\delta(\vec{r}_1 - \vec{r}_2)\right)$, being equal to $(-\ u/L^d)$ and is present only within a small region beyond the Fermi points/ Fermi circle/ Fermi surface i.e outside where the pairing would take place (usual Cooper's model).Then equation (4) reduces to

$$\sum_{\vec{k},\vec{k'}}\{\frac{\hbar^2}{2m}\left[\left(\vec{k}+\frac{\vec{K}}{2}\right)^2+\left(\vec{k}-\frac{\vec{K}}{2}\right)^2+\epsilon\right\}a_{\vec{k}}=C$$

Where

$$C=-u/L^d\sum_{\vec{k'}}a_{\vec{k'}}$$

This leads to

$$a_{\vec{k}}=\frac{-u/L^d\sum_{\vec{k'}}a_{\vec{k'}}}{\{-\frac{\hbar^2}{2m}\left[\left(\vec{k}+\frac{\vec{K}}{2}\right)^2+\left(\vec{k}-\frac{\vec{K}}{2}\right)^2\right]+\epsilon\}} \qquad (5)$$

Now summing over all $\vec{k}$, the constant $\sum_{\vec{k}}a_{\vec{k}}$ appears on both sides. Then we can cast the self consistency condition in the following form,

$$1=u/L^d\sum_{\vec{k'}}\frac{1}{\{\frac{\hbar^2}{2m}\left[\left(\vec{k}+\frac{\vec{K}}{2}\right)^2+\left(\vec{k}-\frac{\vec{K}}{2}\right)^2\right]-\epsilon\}} \qquad (6)$$

The above equation corresponding to zero centre of mass momentum becomes

$$1=u/L^d\sum_{k}\frac{1}{\{\frac{\hbar^2}{2m}2\epsilon_k-\epsilon\}}$$

Now in our case of pairing corresponding to zero centre of mass momentum, in the background of nearest neighbor tight binding 1D or 2D lattice system with Bloch functions acting as the basis functions, equation (4) takes the form:-

$$2a_{\vec{k}}\epsilon_k+\sum_{\vec{k'}}a_{\vec{k'}}V_{\vec{k},\vec{k'}}=\epsilon a_{\vec{k}}$$

leading to $$2\epsilon_k a_{\vec{k}} - \sum_{\vec{k}'} a_{\vec{k}'}\, u/L^d = \epsilon a_{\vec{k}} \qquad (7)$$

Where ϵ_k, the lattice dispersion energy, replaces the free electron energy. L is length and'd' is the dimension of the system. The quantity ϵ_k has the following forms corresponding to i) a nearest neighbor tight binding model and ii) next to next nearest (nnn) neighbor hopping model:-

$$\epsilon_k = \begin{cases} \epsilon_0 - 2t\mathrm{Cos}(ka) & \text{(used for 1D)} \\ \epsilon_0 - 2t\left(\mathrm{Cosk_x a} + \mathrm{Cosk_y a}\right) + 4t'\mathrm{Cosk_x a}.\mathrm{Cosk_y a} - 2t''\left(\mathrm{Cos2k_x a} + \mathrm{Cos2k_y a}\right) & \text{(used for 2D)} \end{cases} \qquad (8)$$

Here 'a' is the lattice constant; t, t', t'' are the single particle hopping parameters corresponding to the nearest, next near neighbour and second next near neighbour respectively on the lattice, ϵ is the two particle energy eigen value as before. $L \to \infty$ for a macroscopic system. It may be remarked that my lattice Hamiltonian for Cooper pairing looks somewhat similar to negative - U Hubbard model, although the attraction here operates only within a finite energy interval. Summing over $\vec{k}$ on both sides of equation (7) and taking the continuum limit, we get for 1D

$$1 = \left(\frac{u}{L}\right)\left(\frac{L}{2\pi}\right)\int_{\tilde{\epsilon}_{\vec{k}\,low}}^{\tilde{\epsilon}_{\vec{k}\,up}} \frac{D(\tilde{\epsilon}_k)d\tilde{\epsilon}_k}{\left(|W| + 2\tilde{\epsilon}_k\right)} \qquad (9)$$

In case of 2D system 'L' will be replaced by L^2 in the above equation.

A new variable $\tilde{\epsilon}_k = \epsilon_k - \epsilon_F$ is introduced here within the standard form of density of states (DOS) where the form of 1D DOS is

$$D\left(\tilde{\epsilon}_k\right) = \frac{1}{2at\sqrt{1 - \left(\frac{\tilde{\epsilon}_k + \epsilon_F - \epsilon_0}{2t}\right)^2}} \qquad (9a)$$

$$\left(\tilde{\epsilon}_{\vec{k}\,up}\right) = \epsilon_F + 4t(1-\delta) + \left(\hbar\omega_{boson} - 4t(1-\delta)\right)\ \theta\left(4t(1-\delta) - \hbar\omega_{boson}\right)$$

$$(\tilde{\epsilon}_{\vec{k}\,low}) = \epsilon_F$$

and 2D DOS takes the form

$$D(\tilde{\epsilon}_k) = K\sqrt{1 - \left(\frac{\tilde{\epsilon}_k + \epsilon_F - \epsilon_0}{2t}\right)^2} \qquad (9b)$$

K is the elliptic integral of first kind.

$$\left(\tilde{\epsilon}_{\vec{k}\,up}\right) = \epsilon_F + 8t(1-\delta) + \left(\hbar\omega_{boson} - 8(1-\delta)\right)\ \theta\left(8t(1-\delta) - \hbar\omega_{boson}\right)$$

$$(\tilde{\epsilon}_{\vec{k}\,low}) = \epsilon_F\,,$$

Here δ is band filling factor. Besides, $|W|$ represents the binding energy of the two electrons with $-|W| = \epsilon - 2\epsilon_F$ for $\epsilon < 2\epsilon_F$, where ϵ_F is the Fermi energy corresponding to a particular filling. It must be emphasized that the quantity $\hbar\omega_{boson}$, is the characteristic energy of the exciton mediating the pairing interaction and is of the order of the band width itself for the Bechhgard salts and cuprates. Therefore very importantly the electronic DOS function has been kept within the integrand in the above equation (9). It is to be noted that this is a very important departure from the original calculations of Cooper, where the calculation was done for a boson, having a very small energy range for attractive interaction above the Fermi surface. Therefore the energy variation of DOS function was completely neglected there. In the next chapters, the non trivial variation of DOS with energy will be shown to lead to realistic consequences, missed out in Cooper's simple treatment.

For marginal Fermi liquid like picture the density of states is

$$D(\omega) = \sum_k -\mathrm{Im}[G(k,\omega)/\pi)/N^2$$

Where

$$G(k,\omega) = \left(\frac{1}{\pi}\right)[1/(\omega - \epsilon_F - \sum(k,\omega))]$$

and N^2 is the number of lattice sites in plane. The above form of the Green's function for a single fermion on the 2D lattice, includes the self energy corrections $\sum(k,\omega)$ to implement the many body effects within the system, where

$$\sum(k,\omega) = \sum^{Re}(k,\omega) + i\sum^{Im}(k,\omega)$$

$$\sum^{Re}(k,\omega) \propto \omega \log\left(\frac{|\omega|}{\omega_c}\right) \text{and} \sum^{Im}(k,\omega) \propto |\omega| \text{for} |\omega| > T$$

We have slightly modified the real part and take it as

$$\sum^{Re}(k,\omega) = g\omega \log((|\omega| + \varepsilon)/\omega_c) \text{for} |\omega| > T, \quad (10)$$

ε is a doping dependent parameter which increases with reduced wave vector. This is associated with the imaginary self energy which is derived by plugging Kramers- Kronig relation viz.

$$\sum^{Im}(k,\omega) = -\left(\frac{1}{\pi}\right)\int_{-\infty}^{\infty}[\frac{\sum^{Re}(k,\omega)d\omega}{(\omega-\omega')}\ ] \qquad (11)$$

Instead of infinite extent the range of the integration is kept limited in between the band width though. We have explicitely checked the applicability of this expression by plotting the real part of self energy against frequency.

Our calculational results corresponding to Cooper pairs with finite centre of mass momentum, are helpful to highlight the spatial nature of the pair wave function [10]. For finite centre of mass momentum in 1D

$$\widetilde{\epsilon}_{k+q/2} = \epsilon_0 - 2t\text{Cos}\left(\vec{k} + \frac{\vec{q}}{2}\right).\vec{a} - \epsilon_F$$

$$\widetilde{\epsilon}_{k+q/2} = \epsilon_0 - 2t\left[\text{Cos(ka)Cos}\left(\frac{qa}{2}\right) \pm \text{Sin(ka)Sin}\left(\frac{qa}{2}\right)\right] - \epsilon_F$$

Depending on the orientation between $\vec{a}$ and $\vec{q}$

$$\widetilde{\epsilon}_{k+q/2} = \epsilon_0 - 2t\left[\text{Cos(ka)} \pm \text{Sin(ka)}\left(\frac{qa}{2}\right)\right] - \epsilon_F$$

Considering $\overrightarrow{|q|}$ to be small compared to $|\vec{k}|$,

$$\widetilde{\epsilon}_{k+q/2} = \epsilon_0 - 2t\text{Cos}(ka) \pm 2t\,\text{Sin}(ka)\left(\frac{qa}{2}\right) - \epsilon_F$$

$$\widetilde{\epsilon}_{k+q/2} = \widetilde{\epsilon}_k \pm atq\,\text{Sin}(ka)$$

Similarly

$$\widetilde{\epsilon}_{k-q/2} = \widetilde{\epsilon}_k \pm atq\,\text{Sin}(ka)$$

Since $\widetilde{\epsilon}_{\vec{k}+\frac{\vec{q}}{2}}$ and $\widetilde{\epsilon}_{\vec{k}-\frac{\vec{q}}{2}}$ are symmetric in $\vec{k}$ space about the minimum of the band, the calculation will be carried out taking just one among them

$$(\widetilde{\epsilon}_{\vec{k}\,up})_{fin} = 4t(1-\delta) - atq\text{Sin}(ka) + (\hbar\omega_{boson} - 4t(1-\delta))\theta(4t(1-\delta) - \hbar\omega_{boson})$$

and

$$(\widetilde{\epsilon}_{\vec{k}\,low})_{fin} = atq\,\text{Sin}(ka)$$

The maximum allowed pairing wave vector 'q_{max}' (defined by $|W|^q = 0$ for $q = q_{max}$) gives us an estimate of the coherence length ('ξ'), which is of the order of reciprocal of q_{max}. However the relation between $|W|$and q here is monotonically decreasing [10].

It may be noted that although $N(\epsilon)$ is a variable here, to have an idea about the strength of the coupling, different values of u/L^d for a particular band filling are multiplied by the DOS at the Fermi energy corresponding to that filling. The expression for the coupling constant (λ) is

$$\lambda = (u/L^d)N(\epsilon_F)$$

At a higher filling the coupling is weaker for a particular pairing energy range, as can be seen in the next chapters, very similar to what happens in the original Cooper's treatment appropriate to 1D.

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3. Pairing in one dimension

This part of my thesis deals with pairing mechanism in quasi one- dimensional systems [1]. In the case of quasi-1D organic superconductors, many important questions came up regarding the pairing mechanism and the nature of the pairing symmetry. As described earlier, I have considered here an electronic excitation mediated mechanism for $(TMTSF)_2X$ salts or Bechhgard salts to examine intra- chain pairing between two electrons in a band, involving singlets character of the pair wave function in a Fermi- sea like background. It must be emphasized however that Bechhgard salts are only considered as possible support for the phenomenological scenario arising from our general formalism and calculations.

The Fermi liquid (FL) model for interacting fermions shows a break down in a purely one-dimensional medium due to the loss of well-defined quasiparticles [2]. The simple decay process of a quasiparticle with wave vector k_1 outside the Fermi sea colliding with a particle in an occupied state of wave vector k_2 inside the sea creates two quasiparticles, wave vectors k_1' and k_2' at low temperature close enough to the Fermi sea. The life time of this excited state is inversely proportional to collision rates [2],

$$\frac{1}{\tau} \propto \sum_{k_2,k_1',k_2'} W(k_1, k_2 \rightarrow k_1', k_2') \times \delta(k_1 + k_2 - k_1' - k_2') \times \delta(\epsilon_{k_1} + \epsilon_{k_2} - \epsilon_{k_1'} - \epsilon_{k_2'}) \times n_{k_2}(1 - n_{k_1'})(1 - n_{k_2'})$$

Here W is the transition probability and the Dirac delta functions represents conservation of (crystal) momentum and energy. The three factors at the end are just the probabilites of the existence of particles and holes involved in the process, excluding the initially free particle. In three dimensions at zero temperature, the life time τ diverges at the Fermi surface, causing the quasiparticles to be well-defined. However, in one dimension, even at zero temperature, the integral is found to yield a life time $\tau = 0$ at the Fermi points. This means that there are no stable quasiparticles, and thus the Fermi liquid theory breaks down. The Luttinger- Tomonaga Liquid LTL) model is constructed to replace FL theory in one dimension. Tomonaga and Luttinger proposed that instead of individual electron motion, the collective motion of fermions involving both spin degrees of freedom and charge degrees of freedom should be treated in terms of harmonic oscillator description to describe the 1-D system [3]. The new quasi-particles emerging

in this theory are of bosonic character, they are 'holons'(having spin zero and charge 'e') and 'spinons'(having spin 1 and charge neutral). In this formalism all the physical quantities are expressed in terms of the charge and spin density operators of fermions, which obey the quantum commutation relation.

The most striking behaviour in LTL theory, is the anomalous power-law dependence of various correlation functions in the low-energy region in the normal phase. For example, the density-density correlation function between two distant positions x and x' exhibits the power-law dependence in the asymptotic region [3]

$$< \rho(x)\rho(x') > \sim e^{2ik_F(x-x')}(x-x')^{-\alpha}$$

The critical exponent α changes continuously depending on the strength of the interaction between particles. Thus the density of states for the LTL at the Fermi energy vanishes like $|E - \epsilon_F|^{\beta}$ (for repulsive interactions) and the jump in the single particle occupation number vanishes as $\sim(k - k_F)^{\alpha}$[3].

Now, the phenomenon of superconductivity occurs in many of these quasi 1-D superconductors at very low temperatures viz. at around 1-2K; whereas the possible applicability of LTL theory to these systems is confined to much higher temperature regime where the inter-chain coupling is broken. For a typical Bechhgard salt, this temperature comes to about 300K. As the occurrence of superconductivity in these systems at low temperature strictly requires the presence of both intra-chain pair formation and inter-chain pair hopping processes as has been discussed earlier, these systems are truly quasi- 1-D like (rather than 1D) in its behaviour particularly at low temperature even in the normal phase as stated previously in the introduction [4]. Therefore, the LTL model description of the normal phase of quasi- 1D superconductors as non-Fermi liquid (NFL) system at high temperature, is not relevant for superconductivity at all [5].

It has been reported that neither the low-energy mode nor the conductivity below the Mott gap observed in experiments in the normal phases of organic superconductors, can be described quantitatively by a simple one-dimensional theory. In a purely 1D theory the conductivity σ_ω should grow as $\sim\omega^3$ in the frequency region between the Drude peak and the Mott peak, however such a power law behaviour is not observed experimentally [6]. In addition, in a doped one-dimensional system the width of the $\omega = 0$ peak should remain extremely narrow since all

electron-electron scattering that can lead to dissipation has been shifted to higher energy [7] . This however contradicts the experimental results.

Soda et al showed that the behaviour of quasi-one-dimensional materials can be classified according to whether the transverse motion is diffusive or coherent. In the former case the material exhibits 1D behaviour (for example, TTF-TCNQ) whereas in the latter it will behave as an anisotropic 3D material (for example, TMTTF-TCNQ) [8,9].

The crossover between these regimes is determined by the criterion

$$\tau_{\parallel} t_{\perp} \sim \hbar$$

where $\tau_{||}$ is the intra- stack carrier lifetime. The crossover condition is satisfied for $(TMTSF)_2PF_6$ at a temperature of 45 K. This crossover temperature is checked and recalculated using the temperature dependence of $\sigma_{||}$ (longitudinal conductivity), which means that at low temperatures at ambient pressure $(TMTSF)_2PF_6$ should have three dimensional characteristics [10]. Therefore the theorems for strictly one dimensional system will not be valid in this kind of material.

The electronic structural configurations of $TMTSF)_2$ X where both ionicity and covalency coexist, may exhibit some anomalous behavior in the optical properties [Reference: Introduction, with subtitle TMTSF salts] . This is manifested in the optical conductivity vs frequency graph of $(TMTSF)_2$ AsF_6 , that shows besides the usual distinct Drude- like peak, an extra hump or peak (in ev range) which may originate from an electronic excitation, as phonons can never acquire such a high energy [11]. Hence the conductivity is described by a non- Drude like functional form $\sigma_0(\omega)$ in addition to the usual Drude one $\sigma_D(\omega)$, characterized by and satisfying the following relations:-

$$\sigma_D(\omega) = \left(\frac{\omega_{pD}^2}{4\pi}\right)\frac{\Gamma_D}{\omega^2 + \Gamma_D^2} \qquad (1)$$

$$\sigma_0(\omega) = \left(\frac{\omega_{p0}^2}{4\pi}\right)\frac{\omega^2\Gamma_0}{(\omega^2 - \omega_{boson}^2)^2 + \omega^2\Gamma_0^2} \qquad (2)$$

$$\int_0^\infty \sigma_D(\omega)d\omega + \int_0^\infty \sigma_0(\omega)d\omega = \frac{\omega_p^2}{8} \qquad (3)$$

Where Γ is the scattering rate of carriers, $\omega_p$is the plasma frequency of the material, ω_{boson} is the position for the non Drude peak, here for $(TMTSF)_2 AsF_6$. Although I have argued in the introduction section that above T ≈ 300K the electronic properties may conform to the LTL description, the standard functional characterization by Fermi liquid (FL) like approach has been carried out by me, to extract the Drude and non-Drude components. This was done by generating the theoretical graph as close as possible to the experimentally obtained one for $(TMTSF)_2 AsF_6$, using the above Drude and non- Drude like expressions and the well known f- sum rule (equation 3) [7].

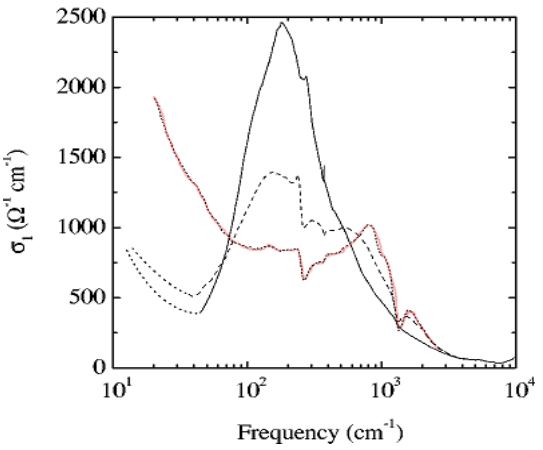

Figure 1.1: Experimentally measured absorptivity of $(TMTSF)_2AsF_6$ vs. frequency, along the highest conducting axis at different temperatures [7]

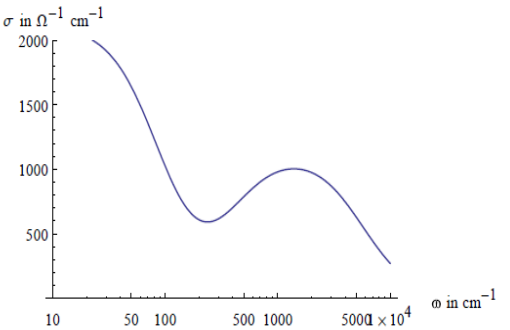

Figure 1.2: Theoretically obtained absorptivity (which is the closest to figure 1.1) of the same material (left) as a function of frequency at 300k.

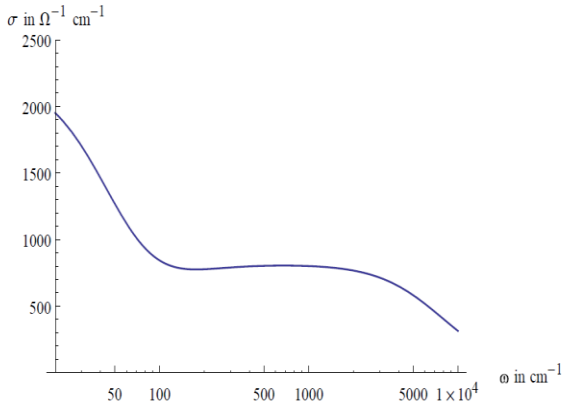

Figure 1.3 : Another example of the theoretically obtained absorptivity of the same material as a function of frequency at 300k

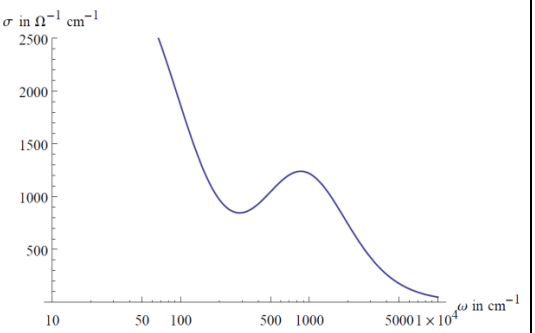

Figure 1.4: Figure 1.4: Another example of the theoretically obtained absorptivity of the same material as a function of frequency at 300k

Figure1. Experimentally measured and theoretically obtained absorptivity of $(TMTSF)_2$ AsF_6

The peak value of the non- Drude portion of the best fitted graph (figure: 1.2) has been identified with ω_{boson} in equation 9(a) of chapter 2: general equation and it has the following values of parameters (as presented in Table 1).

Table1. Values of different parameters extracted for $(TMTSF)_2 AsF_6$ [12]

Theoretical				Experimental
Material	$\hbar\omega_o$ or $\hbar\omega_{boson}$ in cm^{-1}	Effective plasma Frequency from Drude part in cm^{-1} (ω_{pD})	Plasma frequency in cm^{-1} (ω_p)	Plasma frequency in cm^{-1} [12]
$(TMTSF)_2AsF_6$	1050 (0.12 ev)	1449	9061	9900

The spectral weight obtained by integrating the Drude functional form appearing in equation (3) is around 1.6% of the total spectral weight. The extracted bosonic energy value is 0.12 ev; however a small variation in the value of bosonic energy doesn't lead to any qualitative change in our main result.

After performing the integration by parts on the right hand side of equation (9) of chapter 2: general equation we get,

$$1 = \left(\frac{u}{L}\right)\left(\frac{L}{2\pi \times 2at}\right)\left\{\left[\frac{2tSin^{-1}\left(\frac{\tilde{\epsilon}_{\vec{k}} + \epsilon_F - \epsilon_0}{2t}\right)}{\left(|W| + 2\tilde{\epsilon}_{\vec{k}}\right)}\right]_{(\tilde{\epsilon}_{\vec{k}\,low})}^{(\tilde{\epsilon}_{\vec{k}\,up})} + \int_{(\tilde{\epsilon}_{\vec{k}\,low})}^{(\tilde{\epsilon}_{\vec{k}\,up})} \left\{\frac{2}{\left(|W| + 2\tilde{\epsilon}_k\right)^2} \int \frac{d\tilde{\epsilon}_k}{\sqrt{1 - \left(\frac{\tilde{\epsilon}_k + \epsilon_F - \epsilon_0}{2t}\right)^2}}\right\} d\tilde{\epsilon}_k\right\} \quad (4)$$

Now the second part above in the right hand side of equation (4) coincides with a standard form of integration, having two solutions under two different conditions [13]:-

If $a^2 > b^2$, where $a = |W| + 4tCosk_F a$ and $b = 4t$, then

$$\int \frac{\text{arcSinx}\, dx}{(a+bx)^2} = \frac{\text{arcSinx}}{b(a+bx)} - \frac{2}{b\sqrt{a^2-b^2}} \arctan \sqrt{\frac{(a-b)(1-x)}{(a+b)(1+x)}} \qquad (5)$$

(This is referred to as the 1st integral formula throughout the rest of the paper)

and if $b^2 > a^2$ then

$$\int \frac{\text{arcSinx}\, dx}{(a+bx)^2} = \frac{\text{arcSinx}}{b(a+bx)} - \frac{1}{b\sqrt{b^2-a^2}} \ln \frac{\sqrt{(a+b)(1+x)} + \sqrt{(b-a)(1-x)}}{\sqrt{(a+b)(1+x)} - \sqrt{(b-a)(1-x)}} \qquad (6)$$

(This is referred to as the 2nd integral formula throughout the rest of the paper)

The different situations, arising from the above formulae are discussed in the following table

Table 2. Summarized result obtained using 1st (left) and 2nd (right) formula [12]

$a^2 > b^2 \rightarrow \lvert W\rvert^2 + 16t^2Cos^2k_Fa + 8t\lvert W\rvert Cosk_Fa > 16t^2$	$b^2 > a^2 \rightarrow \lvert W\rvert^2 + 16t^2Cos^2k_Fa + 8t\lvert W\rvert Cosk_Fa < 16t^2$
[1]The pairing energy equation according to this criterion is $1 = \left(\frac{u}{L}\right)\left(\frac{1}{\gamma}\right)\frac{-4t}{\sqrt{(\lvert W\rvert + 4tCosk_Fa)^2 - (4t)^2}}$ $\left\{\left[\tan^{-1}\left(\frac{(\lvert W\rvert + 4tCosk_Fa - 4t)\left(1 - \frac{\widetilde{\epsilon}_k - 2tCosk_Fa}{2t}\right)}{(\lvert W\rvert + 4tCosk_Fa + 4t)\left(1 + \frac{\widetilde{\epsilon}_k - 2tCosk_Fa}{2t}\right)}\right)\right.\right.$ $-\left[\tan^{-1}\left(\frac{(\lvert W\rvert + 4tCosk_Fa - 4t)\left(1 - \frac{\widetilde{\epsilon}_k - 2tCosk_Fa}{2t}\right)}{(\lvert W\rvert + 4tCosk_Fa + 4t)\left(1 + \frac{\widetilde{\epsilon}_k - 2tCosk_Fa}{2t}\right)}\right)\right]$ where $\gamma = \frac{4\pi at}{L}$ (7.1)	[1]Pairing energy equation according to this criterion is $1 = \left(\frac{u}{L\gamma}\right)\left(\frac{-2t}{\sqrt{(4t)^2 - (\lvert W\rvert + 4tCosk_Fa)^2}}\right)$ $\times\left\{\ln\frac{\left[\frac{A+B}{A-B}\right]^{\widetilde{\epsilon}_{\vec{k}\,up}}}{\left[\frac{A+B}{A-B}\right]^{\widetilde{\epsilon}_{\vec{k}\,low}}}\right\}$ where $A = \left[\left(4t + \lvert W\rvert - 2(\epsilon_F - \epsilon_0)\right)\times\left(1 + \frac{\widetilde{\epsilon}_k + \epsilon_F - \epsilon_0}{2t}\right)\right]^{\frac{1}{2}}$ $B = \left[\left(4t - \lvert W\rvert + 2(\epsilon_F - \epsilon_0)\right)\times\left(1 - \frac{\widetilde{\epsilon}_k + \epsilon_F - \epsilon_0}{2t}\right)\right]^{\frac{1}{2}}$ and $\gamma = \frac{4\pi at}{L}$ (7.2)
[2]If the filling factor tends to zero then the above inequality turns out to be $\lvert W\rvert^2 + 16t^2 + 8t\lvert W\rvert > 16t^2$. Therefore pairing easily takes place at very low filling with very small value of pairing energy. At the limit of complete filling of the band, this inequality takes the form of $\lvert W\rvert^2 + 16t^2 - 8t\lvert W\rvert > 16t^2$, implying $\lvert W\rvert > 8t$. This implies that the pairing energy will be very high	[2] The above equation shows that to get the desired value of 1 at L.H.S for an infinitesimal u, the rest portion at R.H.S has to be infinite, which is achieved at $\lvert W\rvert \rightarrow 0$, like Cooper case. A very important consequence of my calculations from these above equations (7.1 and 7.2) is that the

and comparable to hopping amplitude at higher filling. Besides, the condition points towards a finite starting value of pairing energy unlike Cooper's original case. Thus we can't get the situation of $\|W\|^0 = 0$ here. The high filling situation is described at point 3 below.	admissible solutions give an upper bound to $\|W\|$. This is in sharp contrast to the continuum case of Cooper, where no such feature is seen.
[3]For having admissible values for the pairing energy equation above, only the following relations involving two sets of $\|W\|$ and $\hbar\omega_{boson}$ are relevant:- 1. $\begin{cases} \|W\| > 4t(1 - Cosk_F a) \\ \hbar\omega_{boson} < 2t(1 + Cosk_F a) \end{cases}$ and 2. $\begin{cases} \|W\| > -4t(1 + Cosk_F a) \\ \hbar\omega_{boson} > 2t(Cosk_F a - 1) \end{cases}$ Besides the simultaneous non vanishing of inverse tangential parts implies 3. $\|W\| + 4tCosk_F a - 4t \neq 0$ and 4. $\begin{cases} 2t(1 + Cosk_F a) \neq \hbar\omega_{boson} \\ 2t \neq -2tCosk_F a \end{cases}$ Inequality 4. is violated at $k_F a = \pi$ implies that at full filling of the band no possibility of pairing exists.	[3]Same conditions or inequalities appear for having admissible values of the pairing energy equation. An important result follows from this inequality viz. $\hbar\omega_{boson} < 2t(1 + Cosk_F a)$ [see inequality (8) on the next page]. This implies a maximum allowed value of Fermi momentum, above which the pairing equation will be non tractable and it also relates a minimum threshold value of $'t'$ for a particular filling and bosonic energy.

3.1 Zero Centre of Mass Momentum:

From the admissible inequalities of Table-2, we have chosen

$$\hbar\omega_{boson} < 2t(1 + Cosk_F a) \qquad (8)$$

to extract some significant physics out. Let us consider, if the band is half filled then $2t > \hbar\omega_{boson}$. In fact for each filling there is a corresponding minimum allowed value of $'t'$, which is determined by the magnitude of bosonic energy. After incorporating the numerical values of parameters viz.'t' (0.25 ev) and $\hbar\omega_{boson}$ (reference Table 1) for $(TMTSF)_2AsF_6$ the same inequality (8) leads to $k_F a < 7/9$ and hence $\delta < 7/9$ (the Fermi points being $\pm k_F$) [14]. Above

this critical filling viz. for $\delta \geq 7/9$ the pairing equation becomes non tractable. It may be noted that real Bechhgard salts exhibit an energy gap due to dimerization at around $\delta \approx 3/4$ and hence is not conducting for $\delta > 3/4$ [15]. So my theoretical results are consistent with this material property, regarding pair formation only in the highest conducting axis and pair transport through the transverse directions.

Based upon the above critical value of the Fermi momentum or filling factor, a distinct division of the whole electronic band can be done into two regions viz. (i) tractable regime and (ii) non-tractable regime. The graphs below are drawn using values of |W|, lower than its upper bound in tractable region, discussed in Table 2, for different values of attractive interaction energy.

Table 3a: Plot of |W| for different values of attractive interaction energy.

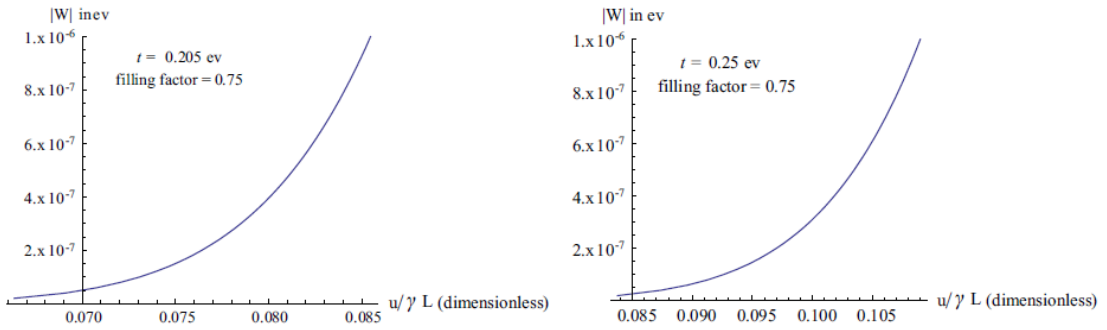

Fig. 2. Plot of |W| vs. dimensionless attractive interaction for two different hopping amplitudes using 2nd integral formula.

The nature of the coupling constant is very similar to that obtained from the original Cooper's treatment appropriate to 1D. At a higher filling the coupling is weaker for a particular pairing energy range, as can be seen in Figures on next page-

Table 3b: Plot of |W| vs. coupling constant

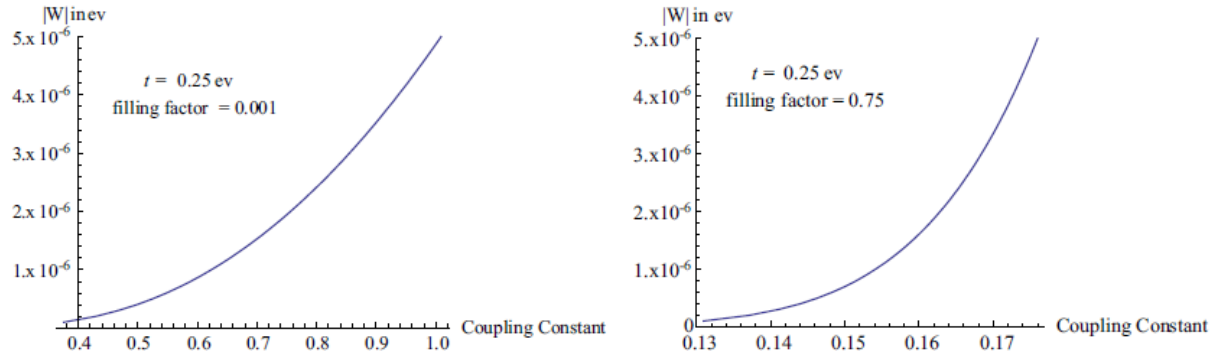

Fig. 3. Graphs separately displaying variation of |W| with coupling constant for different fillings using 2nd integral formula.

Now combining the well known Barden, Cooper, Schrieffer (BCS) theory and Cooper equations corresponding to weak coupling, viz. [16]

$$\frac{2\Delta_0}{KT_c} = 3.5 \qquad (9a)$$

$$kT_c = 1.13\hbar\omega_{boson} \exp\left(-\frac{1}{\lambda}\right) \qquad (9b)$$

and

$$|W| = 2\hbar\omega_{boson} \exp\left(-\frac{2}{\lambda}\right) \qquad (9c)$$

We get

$$\frac{\Delta_0}{|W|} = 0.98875 \times \exp\left(\frac{1}{\lambda}\right) \qquad (9d)$$

Where 'Δ_0' is the superconducting energy gap at zero temperature, the value of which is taken to be of 0.22 mev, obtained from tunneling spectroscopy . '|W|' is the Cooper pair binding energy in 3D isotropic system and 'λ' is the attractive coupling constant. Using these expressions I derived the values of coupling constant and made the following comparison- chart.

Table-4: Comparison between the λ obtained from my calculation and by the conventional method discussed above.

The value of pairing energy (in eV)	Corresponding λ from our graph [pure 1D] (Figure 3)	Corresponding λ obtained by using BCS equation [3D isotropic] (equation 9d)
8.55×10^{-8}	0.13	0.13
2.516×10^{-7}	0.14	0.15
0.97×10^{-6}	0.15	0.19

It should be mentioned here that Ishiguro and co-workers found BCS theory to be consistent for $(TMTSF)_2 X$, while analysing tunneling spectroscopy data [17]. However the usage of these expressions should be quite restricted as these expressions are meant for 3D isotropic BCS system, whereas the experimental system is truly quasi-1D. Also, my calculation is performed here on a one- dimensional lattice, whereas the experimental results for these quasi 1-D systems correspond to a 3D- anisotropic behavior of the superconducting energy gap. Nevertheless, an estimate of the magnitude of the coupling constants obtained from the above two methods are presented in Table: 4 for some general interest and assessment.

3.2 Finite centre of mass momentum

My calculational results corresponding to Cooper pairs with finite centre of mass momentum, are presented below to highlight the spatial nature of the pair wave function in this case. The maximum allowed pairing wave vector 'q_{max}' (defined by $|W|^q = 0$ for $q = q_{max}$) gives an estimate of the coherence length ('ξ') as said earlier in the 'general equation for the pairting instability' chapter. I have presented here two tables relating ξ with different other parameters using the 2nd integral formula. I can't have an assessment of pairing involving finite centre of mass momenta by following the first integral formula, as pairing energy can't be zero in this case (reference: point 1, Table 2). Here too the relation between |W|and q is monotonically decreasing.

Table 5.The calculated values of q_{max} and ξ corresponding to $\delta = 0.001$ under different situations [12]

Value of $\frac{u}{\gamma L} = \lambda$	The corresponding value of |W| (in eV) in case of zero centre of mass momentum	Value of $'t'$ (in eV)	Value of q_{max} (in unit of 1/a)	Value of ξ (in unit of 'a')
0.0012	1×10^{-7}	0.25	3.58×10^{-7}	0.28×10^{7}

Table 6.The calculated values of q_{max} and ξ corresponding to $\delta = 0.75$ under different situations [12]

Value of $\frac{u}{\gamma L} = \lambda$	The corresponding value of |W| (in eV) in case of zero centre of mass momentum	Value of $'t'$ (in eV)	Value of q_{max} (in unit of 1/a)	Value of ξ (in unit of 'a')
0.0881	5.783×10^{-11}	0.35	2.90×10^{-10}	0.345×10^{10}
	8×10^{-7}	0.205	1.5×10^{-6}	0.665×10^{6}
0.17	0.0001	0.25	0.00065142	1535.626536
	0.000811	0.205	0.00584	171.2328767

The magnitude of ξ for higher filling (reference: Table 6) indicates a tendency towards real space like pairing if $'t'$ is reduced progressively (obeying the restriction imposed by inequality 8). This is obvious because the raising of the hopping amplitude weakens the binding of the pair and the mates can now be separated by a larger distance. Hence the coherence length increases. On the other hand increasing of the magnitude of the attractive interaction, causes an enhancement in the pairing energy resulting in reduction in the coherence length.

4. Conclusion:

The non trivial change between the electronic density of states in a lattice and in a continuum system causes several contrasting behaviour between pairing properties in the two situations corresponding to a FL- like scenario. The existence of an upper bound in the pairing energy for 1D lattice is one such example. In addition, the pairing solution also turns out to be band filling dependent in a tricky manner. Finally my calculations show that a realistic fermionic pair formation is indeed possible with some constraints, without any necessity at all of invoking LTL theory. Similarities emerge in the physical properties of the electron pair formed from Cooper's treatment corresponding to continuum and ours, excepting the striking difference appearing in the form of occurrences of a maximum allowed band filling for pairing and of an upper bound of the pairing energy found in our approach [12].

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4. Pairing in Two- Dimension

Among the frontier areas of research in condensed matter physics, the topic of non- Fermi liquid (NFL) occupies an important place. It has been argued that the NFL systems exhibit the phenomenon of the occurrences of Fermi surfaces without long lived quasiparticles. These systems include Luttinger liquid in one- dimension (as has been discussed in introduction and chapter 3) and Marginal Fermi liquid (MFL) in cuprate superconductors [1,2]. A brief introduction of the Luttinger liquid and marginal Fermi liquid has already been done in the previous chapters. However, the microscopic origin of MFL behaviour of the self-energy has remained an open problem. It is worth emphasizing that extraction of the self-energy from experiment is not only of great importance to check the validity of the quasiparticle concept and understand the nature of interactions involved but also is an extremely difficult task. By causality, the real and imaginary parts of self-energy are related by Kramers-Kronig dispersion relations. In principle, if the full spectral function A(k, ω) is known, one could perform an inversion to obtain the full self energy spectra by using the Kramers-Kronig transformation [3] . However, such transformation has limitations and requires the spectrum from $-\infty$ to $+\infty$ in energy. Unfortunately, clean ARPES data from doped cuprates can usually be obtained from Fermi level to around half of the band width where complications of valance bands will come in. So the process requires further to take a cut-off/extension model at energies above the existing data points. A large number of theoreticians are involved in investigations to better understand the normal state scattering rate, which governs the transport properties, but there are serious limitations. They measure or infer the scattering rate ($\sum^{Im}$) at a single energy (ω) and do not extract its functional form. Other studies that investigate the scattering rate as a function of energy are limited to the nodal direction alone. The data presented in my paper provide a comprehensive measurement of the functional form of the scattering rate as a function of energy around the Fermi surface [4].

So I am revisiting Cooper's formalism for fermionic pairing for overdoped cuprates involving two next near neighbour hopping terms in Fermi liquid like background on a lattice. Then the whole scheme is repeated in Marginal Fermi liquid- like background, taking the self energy correction of the Green's function to include a more realistic density of states in the calculation. My formalism promotes and sysnthesizes the Marginal Fermi liquid- like character of the lightly overdoped normal phase with exciton mediated pairing in the concerned materials.

I have done my calculation for studying the possible pairing between two fermions in both Fermi liquid- like and Marginal Fermi liquid- like backgrounds with phononic mechanism as well as excitonic mechanism [4]. I extract various important physical quantities for cuprate superconductors, such as coherence length, coupling constant and critical temperature. After a careful quantitative comparison of my theoretical results with the experimental ones, I have arrived at the strong conclusion of the existence of the electronic mechanism driven pairing from MFL like normal phase in the lightly overdoped cuprates. Theoretical demonstrations justifying the substantial s-wave component and experiments with Raman scattering and tunneling spectra back the conception of a sturdy existence of s- wave symmetry along with other pairing symmetry [5]. I have examined the adequacy and feasibility of the s- wave symmetry in intra-layer pair formation though the presence of a d-wave symmetry is not ruled out.

Mathematical Formalism:

The analogous form of pairing equation including the highly asymmetrical energy dispersion relation in two dimensional tight binding hamiltonian by Cooper's treatment reads as (mentioned in chapter 2, equation 9b) [6]:

$$\left(\frac{u}{A}\right) = U = \frac{1}{\int_{\epsilon_F}^{\epsilon_F + 8t(1-\delta)+(\hbar\omega_{boson}-8t(1-\delta)\theta(8t(1-\delta)-\hbar\omega_{boson})} \frac{D(\tilde{\epsilon}_k)\, d\tilde{\epsilon}_k}{(2\epsilon_k - 2\epsilon_F + |W|)}} \qquad (1)$$

The equation (1) represents the pairing situation in the 'passive Fermi Sea' background. Now to examine the realistic concept of pair formation in the presence of an active Fermi sea, I have to include the effect of Pauli's exclusion principle or rather Pauli blocking of the phase space. For this a factor $1 - f_{-k} - f_k$ has to be incorporated in the 2D single pairing equation. For the finite centre of mass momentum $\hbar q$ this equation takes the form in the following way-

$$1 = U \sum_{\vec{k}} \frac{1 - f_{-k+q/2} - f_{k+q/2}}{-\epsilon + 2\epsilon_F}$$

where $f_{k+q/2}$ is the probability that there is a carrier of momentum $k + q/2$ above the Fermi level. This leads to following equation→

$$1 = U\sum_{\vec{k}} \frac{-1+\theta\left(\epsilon_{k+\frac{q}{2}}-\epsilon_k\right)+\theta(\epsilon_{-k+\frac{q}{2}}-\epsilon_k)}{\left(|W|+2\tilde{\epsilon}_k\right)} \qquad (2)$$

The characteristic of the Theta function determines the range of pairing and finally the pairing equation corresponding to this 'active Fermi sea' background becomes [4]:

$$\left(\frac{u}{A}\right) = \left(\frac{\pi^2 B}{2}\right) \frac{1}{-\int_0^{\hbar\omega_{boson}} \frac{K\sqrt{1-\left(\frac{\tilde{\epsilon}_k+\epsilon_F-\epsilon_0}{2t}\right)^2}\,d\tilde{\epsilon}_k}{\left(|W|+2\tilde{\epsilon}_k\right)} + \int_{atqSin(ka)}^{\hbar\omega_{boson}} \frac{K\sqrt{1-\left(\frac{\tilde{\epsilon}_k+\epsilon_F-\epsilon_0}{2t}\right)^2}\,d\tilde{\epsilon}_k}{\left(|W|+2\tilde{\epsilon}_k\right)} + \int_{-atqSin(ka)}^{\hbar\omega_{boson}} \frac{K\sqrt{1-\left(\frac{\tilde{\epsilon}_k+\epsilon_F-\epsilon_0}{2t}\right)^2}\,d\tilde{\epsilon}_k}{\left(|W|+2\tilde{\epsilon}_k\right)}} \qquad (3)$$

It may be remarked that our lattice Hamiltonian for Cooper pairing looks somewhat similar to negative - U Hubbard model, although the attraction here operates only within a finite energy interval. It may be remarked here that to start with we keep both the possibilities of bosonic mechanism viz. electronic and phononic open under s-wave pairing scheme. For the MFL scenario

$$D(\omega) = \sum_k -Im[G(k,\omega)/\pi)/N^2 \qquad (4)$$

$$\text{Where } G(k,\omega) = [1/(\omega - \epsilon_k - \sum(k,\omega))] \qquad (5)$$

The above form of the Green's function for a single fermion on the 2D lattice, includes the self energy corrections $\sum(k,\omega)$ to implement the many body effects within the system. Researchers in general parameterize only ARPES data and suggest various models of self energy consistent with the fitted plots [7-10]. As mentioned earlier I have slightly modified the real part expression of the self energy as proposed by Varma and take it as

$$\sum^{Re}(k,\omega) = g\omega \ln\left(\frac{|\omega|+\varepsilon}{\omega_c}\right) \text{for } |\omega| > T, \qquad (6)$$

'g' is a real number. 'ε' is a doping dependent parameter which increases with reduced wave vector. $\sum^{Re}(k,\omega)$ is associated with the imaginary self energy which is derived by plugging Kramers- Cronig relation viz [3].

$$\sum^{Im}(k,\omega) = -\left(\frac{1}{\pi}\right)\int_{-\infty}^{\infty}[\frac{\sum^{Re}(k,\omega)d\omega}{(\omega-\omega')} \qquad (7)$$

Instead of infinite extent the range of the integration is kept limited in between the band width though. I have explicitely checked the applicability of this expression by plotting the real part of self energy against frequency. This small change in the proposed MFL self energy formula and the associated parameterization gives an almost accurate matching for the ARPES spectra obtained from Bi2212 sample [11].

Fig 1: A small remodeling of the MFL self energy has been done on the basis of analysis of line shape spectra in Bi2212 sample.

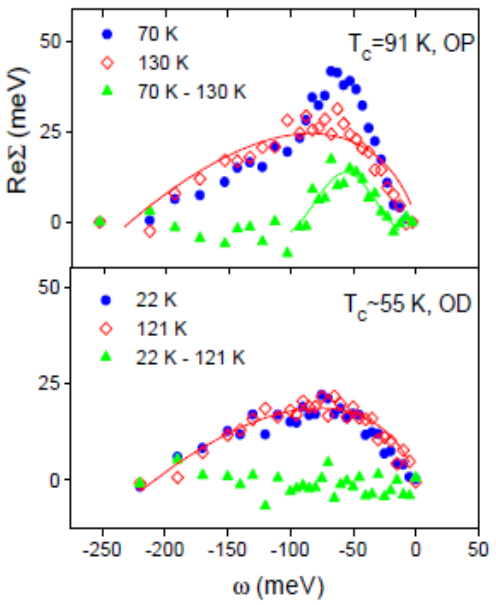

Fig: 1a Real part of self energy as a function of energy for the superconducting (blue dots) and normal states (open red diamonds) for the optimally doped and overdoped samples, as obtained by reference indicated [11]. The solid lines through the normal state data represent MFL fits to the data.

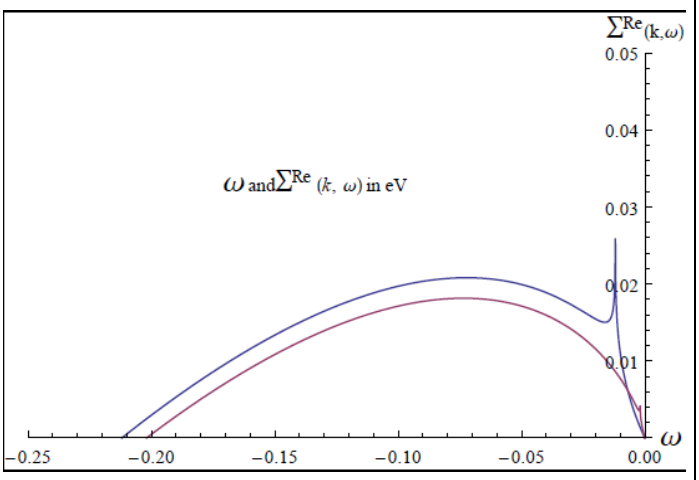

Fig: 1b Remodelling of $\sum^{Re}$ using our formula for Bi2212. The red line (below one) is for overdoped and the blue line (above one) corresponds to optimally doped region.

The corresponding imaginary part of self energy viz. $\sum^{Im}(k, \omega)$ is obtained by incorporating the form of real part of self energy (from fig 1b) in Kramers Kronig relation in a full band width and is parameterized with the following function of ω, to be incorporated in the Green's function.

$$f(\omega) = \left(-.1129\sqrt{1.015 - 5(\omega - .03)^2}\right) \qquad (8)$$

Here are the two plots for this function.

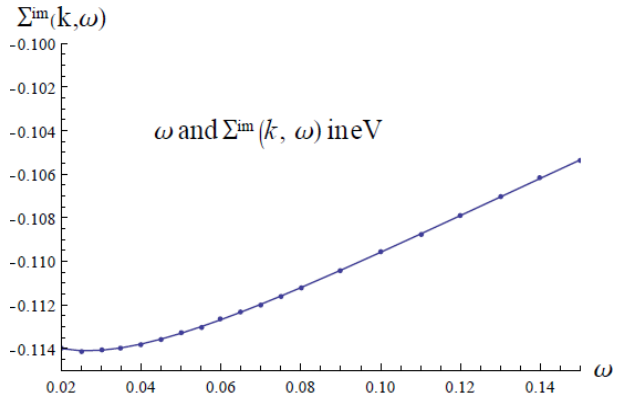

Figure 2a:
Graph of Imaginary self energy values obtained from the Kramers-Kronig relation

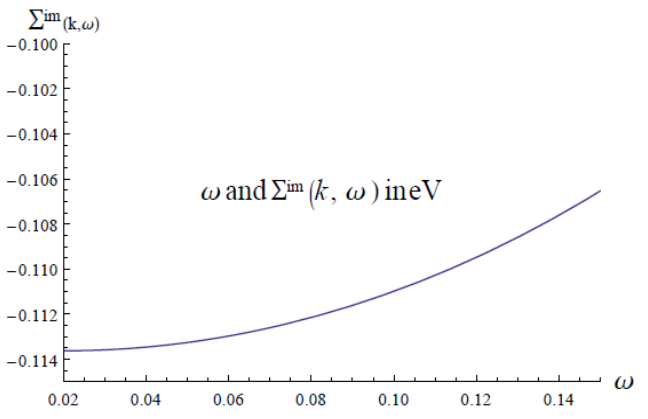

Figure 2b:
Plot of corresponding function that parameterizes the discrete points of the graph at left.

The fitting of imaginary self energy is quite tricky as it is considered to be linear with frequency but shows a visible deviation from linearity as obtained from different spectroscopic experimental result [7-10]. My graph shows a hyperbolic nature of $\sum^{Im}(k, \omega)$ as a function of ω, but behaves almost linearly over a large frequency region. The data presented in my paper provide a comprehensive measurement of the functional form of the scattering rate as a function of energy around the Fermi surface. More importantly, my form for $\sum^{Im}(k, \omega)$ obtained from Kramers-Kronig relation (Figure 2a) shows a noticable qualitative similarity with those extracted from ARPES [7-8]. On the next page there are some ARPES graphs which more or less deviate from the standard linear nature of the imaginary self energy with frequency (Figs. 3a-3d) [7-10].

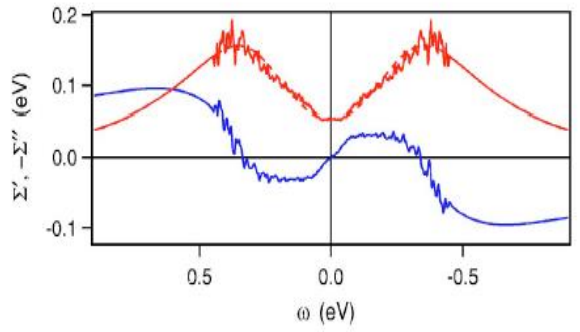

Figure 3a:
The results of the fitting procedure for Bi(Pb)-2212 OD75: for real and imaginary parts of the self-energy [7].

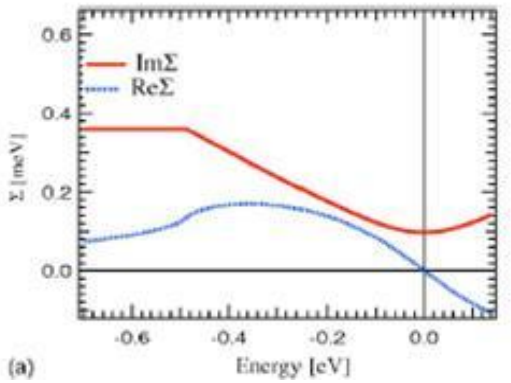

Figure 3b:
The fitting of the EDC (energy distribution curve) data for the energy dependence of the scattering rate of the high temperature cuprate superconductors obtained from angle resolved photoemission spectroscopy [8].

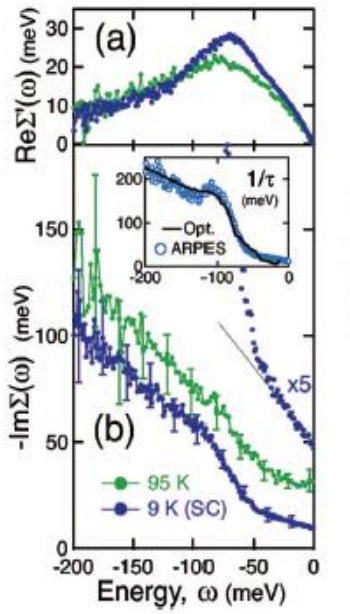

Figure 3c:
Real part and imaginary part of self energy as obtained by angle-resolved photoemission spectroscopy for overdoped cuprates [9].

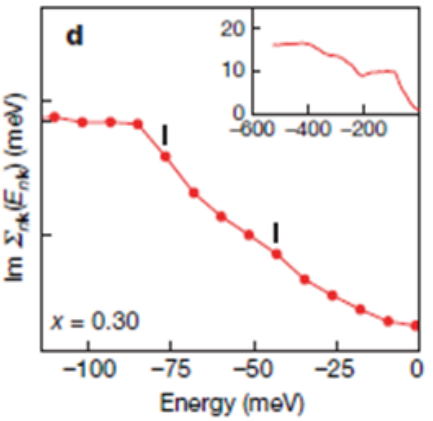

Figure 3d:
Calculated imaginary part of self energy for overdoped LSCO from ARPES data.[10]

The density of states (DOS) associated with the total self energy of the following form is plotted below [12]. Therefore the total self energy takes the form

$$\sum(k,\omega) = \sum^{real}(k,\omega) + i\sum^{im}(k,\omega)$$

$$= \left\{ 0.24\left(\omega \ln\left[\frac{\text{Abs}[\omega + .012]}{.2}\right]\right) + i\left(-.1129\sqrt{1.015 - 5(\omega - .03)^2}\right)\right\}$$

$$/200^2 \qquad (9)$$

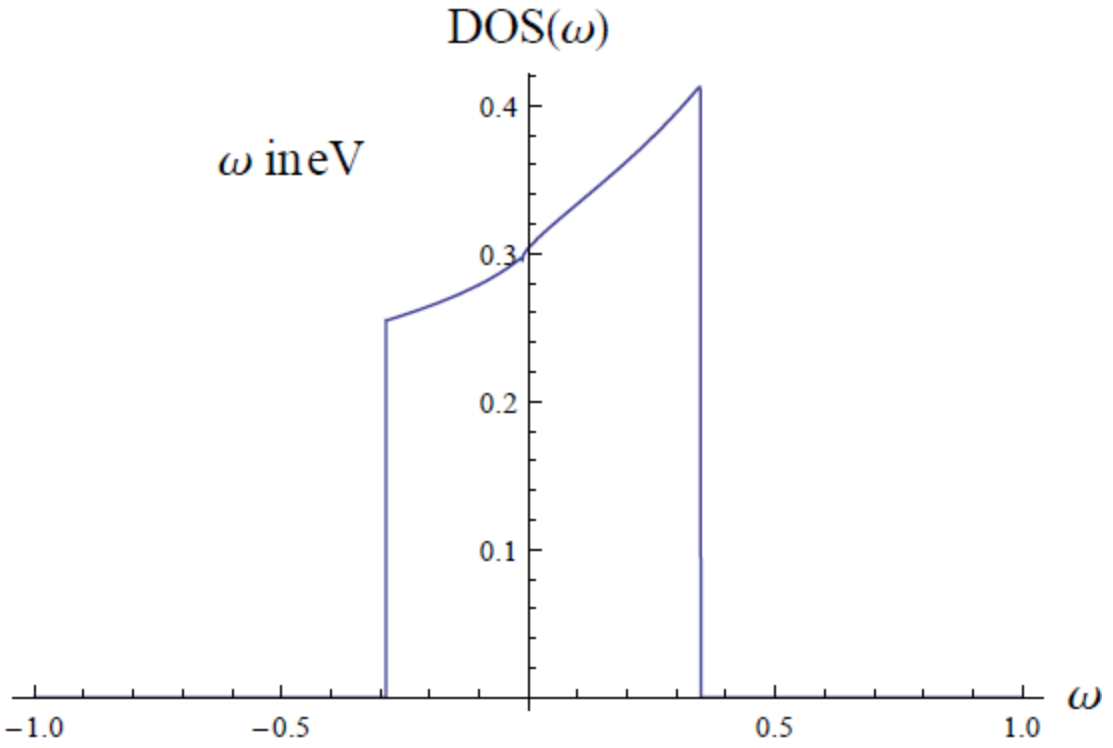

Figure 3 Plot of density of states vs energy using our theoretical expression of self energy

It must be kept in mind however, that the pairing equation is strictly not valid at $\omega = \epsilon_F$ as the quasi particle weight vanishes there [13]

In my formalism the band is completely empty (i.e filling factor δ=0) when doping concentration is 100%. Then introduction of carrier raises the degree of band filling with δ=1 representing half filled band. So the lower portion and the very upper portion of the band represents extremely overdoped and extremely underdoped region respectively as per the phase diagram (ordering temperature vs doping concentration) of the cuprate superconductors [14]. The region in between

these two represents optimally to moderately overdoped region where superconductivity is likely to occur. The attractive coupling constant (λ) has been calculated using the formula [6]

$$\lambda = \left(\frac{u}{A}\right) D(\epsilon_F) \qquad (10)$$

The idea of the coherence length comes out clearly by understanding the spatial nature of the pair wave function associated with the finite centre of mass momentum case. The maximum allowed pairing wave vector 'q_{max}' (defined by $|W| = 0$ for $q=q_{max}$) gives an estimate of the coherence length ('ξ'), which is of the order of reciprocal of q_{max}. The finite centre of mass momentum analogue of the pairing equation is

$$1 = u/A \sum_k \frac{1}{\{(\epsilon_{k+\frac{q}{2}} + \epsilon_{-k+\frac{q}{2}}) - \epsilon\}} \qquad (11)$$

With $\epsilon_{k+q/2} + \epsilon_{-k+q/2} = 2\epsilon_k + 2t'(aq)^2 \mathrm{Sin}(k_x a)\mathrm{Sin}(k_y a)$

The upper and lower limit of ϵ_k has been modified into

$$\epsilon_F + \hbar\omega_{boson} - t'(aq)^2 \mathrm{Sin}(k_x a)\mathrm{Sin}(k_y a)/2 \text{ and } \epsilon_F + t'(aq)^2 \mathrm{Sin}(k_x a)\mathrm{Sin}(k_y a)/2 \qquad (12)$$

Calculations and results:

Scanty experimental data leads to an ambiguity in the energy of the boson, mediating pairing. I get good and realistic result in the range of 0.1- 0. 2 eV which in general is catagorised under electron originated pairing mechanism [15]. It may be remarked that a vertex correction can become quite important in the first principle calculation for 'u' if the bosonic energy (specially relevant for excitonic boson) becomes comparable to the Fermi energy, which is not the case here [16].

Both phononic and excitonic energy value has been incorporated in the pairing equation as the bosonic energy mediating pairing to check the substantiality of these two .The whole calculation is done in such a manner so that the basic Fermi Liquid- like criterion ($u< 4t$) is maintained. The relevant parameters presented in Table-1 are quite realistic [17].

Table-1: Parameters corresponding to pairing mechanism

Parameters	Electronic mechanism	Phononic mechanism
Bosonic energy ($\hbar\omega_{boson}$)	0.1-0.2 eV	0.01-0.02 eV
t	0.435 eV	
t′	0.1 eV	
t"	0.039 eV	

FL like scenario:

The estimates for coherence length obtained in this case, is presented in the Table below

Table 2: The calculated values of coherence length of Bi2212 for u/A=1 eV

	Electronic mechanism		Phononic mechanism	
δ	Value of ξ (in unit of 'a')	Value of T_C	Value of ξ (in unit of 'a')	Value of T_C
0.25	116.28	27.06	-	-
0.5	39	90	117.64	3
1	38	100	149.25	7.07
1.15	143	22.58	-	-
1.3	333	10.48	-	-

Generally real high- T_c cuprates (both in the under and overdoped regions) have short in-plane coherence length [18]. My theoretical estimates (shown in Table 2) point to the fact that

1) The in- plane coherence lengths corresponding to excitonic mechanism are much shorter than those in the conventional phonon driven 3D superconductors. The values of critical temperature in phononic mechanism are not realistic too. Lowering of the magnitude of coherence length or enhancement of critical temperature in the filling factors other than δ =0.5 and 1 needs a large increase in the phonon mediated attractive interaction. This would violates the FL scenario and make it inappropriate for the overdoped phase.

Therefore, the excitonic mechanism is the most feasible one for intra- layer pairing in the overdoped regime [4].

2) The above calculations show the most realistic signature of pairing in moderately overdoped (intermediate band filling range namely δ= 0.5-1) region. The coherence length is smallest and in the vicinity of half filling. Otherwise it is too long to be realistic.

But the coherence length is not of the order of experimental value with FL like description for the normal phase. According to the Table 2, the smallest coherence length is around 145 Å (38 lattice spacing) which is two or three times greater than the experimentally obtained value of coherence length.

If I try to look into the practical significance of this result then I recall that as per the experimental phase diagram of cuprate superconductors the underdoped normal regime doesn't obey the FL theory and superconductivity breaks down in extremely overdoped region [14]. The non- feasible result regarding the coherence length in the upper and lower phase of band beyond a particular filling factor with FL background indicates an unrealistic situation for pairing in underdoped and extremely overdoped regime upholding the phase diagram. So following the above result obtained from FL- like scenario, I now do my calculation in MFL like scenario with excitonic mechanism based pairing in the intermediate band filling range.

MFL- like scenario:

Table-3: Parameters corresponding to pairing in Bi2212 for a filling factor δ=0.99

Bosonic energy	Value of u/A=1.14 eV	Parameters	Values
0.1 eV	1.28	Coupling Constant (λ)	0 .44352
		Coherence length (in unit of lattice constant)	14.28 a
		Temperature	85.76K
0. 15 eV	1.14	Coupling Constant (λ)	0 .4
		Coherence length (in unit of lattice constant)	17.85 a
		Temperature	90K

Strikingly the values of these three definitive signatures of overdoped cuprates -1) Short in-plane coherence length 2) Strong coupling constant and 3) High critical temperature are very much consistent with the experimentally obtained data for the relevant materials [19]. The qualitative result regarding the change of coherence length with the filling factor remains same as for the FL like description for the normal phase.

The critical temperature is the temperature correspondence of |W| which was extracted from the conventional Cooper's and BCS equations corresponding to the isotropic 3D case [20].

$$|W| = 2\frac{(KT_c)^2}{(1.13)^2\hbar\omega_{boson}} \qquad (13)$$

I however consider the usage of the equation (13) here to be very limited as this is appropriate for 3D isotropic system, whereas our calculation is done in 2D. Nevertheless, we still compare the estimates of the coupling constant from the two approaches. Analysis of the available experimental results from Angle Resolved Photoemission Spectroscopy (ARPES) and from polar angular magnetoresistance oscillations show the presence of a 3D coherent electronic behaviour in overdoped phases of some of the cuprate superconductors. Investigation of the oscillations shows that at certain symmetry points however, the Fermi surface exhibits properties characteristic of 2D systems[21]. This striking form of the Fermi surface topography, provides a natural explanation for a wide range of anisotropic properties both in the normal and superconducting states of this system.

The other two parameters (λ and ξ)are derived numerically by using the pairing equation. The coupling constant lies in the range, i.e. λ~0.4 for Bi2212 and coherence lengths are of the order of 10^{-1} Å conforming to experimental values of till date [18].

In Cooper's model in continuum or in BCS Theory $'\lambda'$ is independent of $\hbar\omega_{boson}$. According to McMillan's equation (obtained by simplification of Elliashberg's equation) however λ is inversely proportional to $\hbar\omega_{boson}$ [22]. This is in qualitative agreement with the variation seen in Table 3.

Conclusion and Discussion:

My calculations following a MFL- like description of the normal phase with boson mediated pairing, reproduces real physics regarding the coherence length, coupling constant and critical temperature of the cuprate superconductors in general agreement with more sophisticated many body treatments like Eliashberg scheme and with experiments on real superconductors more sensitively than by FL like description does [4]. From this viewpoint, the MFL like scenario with electronic mechanism seems to be more feasible one for the pairing in cuprates [23].

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Future Plan:

1) Since ξ calculated for quasi 1- D Bechhgard salts is an intra-chain parameter, it is difficult to obtain the corresponding three dimensional result directly. For that both intra- chain pairing and inter- chain pair hopping processes will have to be considered explicitly, so that the anisotropy of the system is incorporated while describing the process leading to superconductivity. I have confined my analysis only to the particle particle pairing channel in a single electronic band. The possibility of existence of fermionic pair states or fermionic truly bound states within the forbidden bands (both above and below the band under consideration) is itself a very challenging problem and needs detailed investigation in future. A more detailed and intricate calculation involving dielectric function extracted from $\sigma(\omega)$ and with inclusion of longitudinal modes will be carried out as a future project.

2) Also I am interested to work on d- wave symmetry involved pairing in cuprate superconductors in both underdoped and overdoped regime.