Chapter One

Introduction

1.1. Brief history:

The phenomenon of superconductivity, in which the electrical resistance of certain materials completely vanishes at low temperatures, it is one of the most interesting and sophisticated in condensed matter physics. The Dutch physicist Heike Kamerlingh Onnes, who was the first to liquefy helium (which boils at 4.2 Kelvin at standard pressure), first discovered it. In 1911, Kamerlingh Onnes and one of his assistants discovered the phenomenon of superconductivity while studying the resistance of metals at low temperatures. They studied mercury because very pure samples could easily prepared by distillation [1].

Low temperature superconductivity accounts for s-wave pairing. Unconventional superconductivity has a popular field in condensed matter physics. It started with the study of super fluid helium, where the order parameter has p-wave symmetry. Later on, several superconducting heavy fermions compounds such as $CeCu_2Si_2$ or UPt_3 found to have an unconventional symmetry of the order parameter. In recent years the interest has risen again due to the discovery of d-wave superconductivity in hole-doped high temperature (high-T_c) superconductors as $YBa_2Cu_3O_7-$ (YBCO) or $BiSr_2Ca_2Cu_2O_{10} -$ $(BSCCO)$. Sr_2RuO_4, discussed to exhibit a p-wave or even an f-wave symmetry of the order parameter [2].

1.2. The aim of the study:

Study the mechanism of d-wave superconducting properties at high temperatures.

1.3. The problem of the study:

The main problem of d-wave superconductivity there is no generally accepted microscopic model to describe this mechanism.

1.4. Literature review:

Different attempts used to describe low energy model of a d-wave superconductor, and describe how self-energy corrections applied to the single-particle and two-particle Green's functions [3].Some researchers also studied the case for $d_{x^2-y^2}$ pairing in the cuprate superconductors and discussed the pseudogap and pairing mechanisms [4].

1.5. The presentation:

This research consists of four chapters; the first explains the introduction, the aim of the research, the research problem and literature review and the second chapter basic concepts of superconductivity. While the third chapter deals with the theory of high temperature superconductivity and shows the last chapter d-wave symmetry.

Chapter Two

Basic Concept of Superconductivity

2.1. Introduction:

Superconductors have the ability to conduct electricity without losing of energy. When current flows in an ordinary conductor (copper wire), some energy is lost. As the superconducting electrons travels through the conductor they pass unobstructed through the complex lattice, because create no friction, they can transmit electricity without loss in the current and no loss of energy [5].

2.2. Properties of superconductivity:

- Zero resistance: no resistance is detectable even for high scattering rates of conduction electronic.

- Absence of thermoelectric: no seebeck voltage, no Thomson heat is detectable.

- Ideal diamagnetism: $x = -1$ weak magnetic fields are completely away from the superconductor [6].

2.3. Types of superconductors:

2.3.1. The first type (Soft superconductors):

Type 1 superconductor or superconductor of the first kind, expels the magnetic field up to maximum value BCS, the critical field for larger fields superconducting break down. The critical field depends on the temperature and reaches zero at the transition temperature T_c, example of type – I superconductor mercury [7, 8].

2.3.2. The second type (Hard superconductors):

Some metallic alloys become superconducting at low temperatures, but they show different behaviors in magnetic fields. Materials with this behavior called "type II" superconductors. Within the range $H_{c1} <$ H $< H_{c2}$, normal and superconducting states exist in this type of superconductors. Type II superconductors normally have much higher critical fields and therefore could carry much higher current densities while remaining in the superconducting state [7].

2.4. The BCS theory:

The understanding of superconductivity advanced in 1957 by three American physicist's john Bardeen, Lean Cooper and John Schrieffer, through their theories of superconductivity, known as the BCS theory. The BCS theory explains superconductivity at temperatures closed to absolute zero [9].

We present below some physical arguments and ideal underlying this theory.

2.4.1. Cooper pair:

Cooper pair is a pair of electrons (or other fermions) bound together at low temperature, in a certain way. Cooper pair is quantum effect, the electron is repelled from other electrons due to their negatives charge, but it also attracts the positive ions that make up the rigid lattice of the metal [10].

2.4.2. Interaction between electrons and phonons in Cooper pairs:

On collision with a phonon, an electron wave vector K absorbs the phonon takes up its energy hv_q and scattered into a nearby state of wave vector $K^{'}$. The electron has absorbed heat from the lattice and is now in a quantized state of different energy. The energy conserved in the process so that the new energy $E(K^{'})$ of the electron is the sum of its former energy $E(K)$ and that hv_q of the absorbed phonon:

$$E(K^{'}) = E(K) + hv_q \tag{2.1}$$

When the electron absorbs the phonon, it also takes up its momentum and changes its direction.

$$\hbar K + \hbar q = \hbar K', \quad K + q = K' \tag{2.2}$$

The conservation of momentum leads to

$$K^{'} = K - q. \tag{2.3}$$

Indeed an electron moving through a lattice considered as continuously emitting and absorbing phonons: it is "clothed" with virtual phonons. Virtual states can think about in terms of the Heisenberg uncertainty principle in the form $\Delta E \Delta t \approx \hbar$. Electron-virtual phonon processes play a central role in the development of the superconducting state. An electron in a state K_1 near the Fermi surface emits a virtual phonon q and scatters into a state K'_1. The law of conservation of momentum requires that for this process:

$$K'_1 = k_1 - q \tag{2.4}$$

Another electron in a state K_2 absorbs the virtual phonon and scattered to a state K'_2 that defined as:

$$K'_2 = K_2 + q \tag{2.5}$$

From equations (2.4) and (2.5) above:

$$K_1 + K_2 = K'_1 + K'_2 = K \tag{2.6}$$

Here K is the total momentum of the pair. In this principle, the interaction between the electrons may be either repulsive or attractive, the determining factor being the relative magnitudes of the phonon energy hv_q and the energy difference between the initial and final states of the electrons. For bonding between electron pairs to occur, the net attractive potential energy$(-v_{ph})$ arising from virtual phonon exchange must be larger than the Columbic repulsive energy (v_{rep}) between the electrons. Therefore, using the convention that a negative potential energy gives rise to attractive forces, the energy balance being:

$$-v_{ph} + v_{rep} < 0 \tag{2.7}$$

2.4.3. Existence of energy gap:

Cooper pairs are bound together by a very small energy, and from a new ground state which is superconducting and is separated by an energy gap, 2Δ, from the next lowest excited state above it [11].

2.5. London theory:

In 1935, Fritz and H. London proposed the following equations to govern the microscopic electric field, E, and magnetic field, B in superconductors. They postulated that a fraction of electrons n_s called the superconducting fraction, exhibit perfect conductivity, while the reminder-the normal fraction denoted by a subscription n-exhibited regular ohmic dissipation [12].

The current density given by:

$$\frac{\partial j_s}{\partial t} = \frac{n_s e^2 E}{m}, \quad J_n = \sigma_n E \tag{2.8}$$

Where E the electric field and σ_n is the electrical conductivity for metals.

The electron densities as

$$n_s(T) + n_n(T) = n$$

$$\nabla \times J_s = -\frac{n_s e^2}{m_{sc}} B \tag{2.9}$$

Where m_{sc} mass of electron in superconductor state and e charge of electron and B the magnetic field.

Now taking the curl of the Maxwell equation, assume that in equilibrium there is no current carried by the normal component as

$$\nabla \times B = \frac{4\pi}{C} J_s \tag{2.10}$$

$$\nabla^2 B = \frac{4\pi n_s e^2}{mc^2} B = \frac{1}{\lambda^2} B \tag{2.11}$$

When the London penetration depth (λ_l) defined as:

$$\lambda_l = (\frac{mc^2}{4\pi n_s e^2})^{\frac{1}{2}} \tag{2.12}$$

$$B(x < 0) = B_0 e^{\frac{x}{\lambda_l}} \tag{2.13}$$

2.6. The Ginzburg-Landau theory:

In 1950, Ginzburg and Landau proposed a theory based on Landau's general theory of second order phase transitions. The superconducting electrons described by a complex wave function,ψ, such that $n_s = |\psi|^2 = \psi^* \psi$ by expanding the expression for the free energy, a differential equation derived of ψ:

$$\frac{1}{2m}(-i\hbar\nabla + 2\text{eA})^2\psi + (\alpha + \beta\psi\psi^*)\psi = 0 \tag{2.14}$$

The super current density given by:

$$J_s = \frac{ie\hbar}{m}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{4e^2}{m}A\psi\psi^* \tag{2.15}$$

Where A is the magnetic vector potential such that $B = Curl\ A$.

The Ginzburg-Landau equations lead to two characteristic lengths, the G-L penetration depth, λ_{GL} as

$$\lambda_{GL} = \sqrt{(m\beta/4\mu_0 e^2 \alpha)} \tag{2.16}$$

And the coherence length, ξ equal

$$\xi = \sqrt{(\hbar^2/2m\ \alpha)} \tag{2.17}$$

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Where α is proportional to $(T - T_c)$ and β is independent of T.

This penetration depth is, like the London penetration depth. The coherence length described as the length scale over which the order parameter varies. As both λ_{GL} and ξ are inversely related to α, they are dependent on temperature and both diverge as T approaches. However, the ratio of the parameters as

$$K = {\lambda_{GL}}/{\xi} \qquad (2.18)$$

Which was known as the Ginzburg-Landau parameter, does not depend on α and therefore approximately independent of temperature [8, 12].

2.7. Flux Quantization:

London in 1950 speculated that the magnetic flux passing through a superconducting ring or a hollow superconducting cylinder can have values equal to ($\frac{nh}{e}$) where n is integer. The flux Quantization confirmed experimentally but the quantum of flux has been found to be ($\frac{h}{2e}$) rather than ($\frac{h}{e}$). By stock theorem:

$$\int A.\,dl = \oint(\nabla \times A).\,ds = \int B.\,ds = \emptyset \qquad (2.19)$$

Where $\emptyset$ is the flux enclosed by s is the area defined by

$$\oint \nabla\delta.\,dl = \Delta\delta = 2\pi n$$

$$\emptyset = \frac{nh}{2e} = n\emptyset_0 \qquad n = \ (0,1,2,\dots) \qquad (2.20)$$

Where $\emptyset_0$ unit of flux called fluxoid and is nearly equal to 2.0676 gauss.cm^2 [10].

2.8. The Josephson effects and tunneling

Josephson observed some remarkable effects associated with the tunneling of superconducting electrons through a very thin insulator (1-5nm) sandwiched between two superconducting, such on insulating layer forms a weak link between the superconductors which is referred to as the Josephson junction. The Josephson current is proportional to the sin of the phase difference ($\emptyset_1 - \emptyset_2$) of the macroscopic wave function of the two superconductors [10]. We have:

$$I_s = I_c sin\gamma \tag{2.21}$$

Where γ is the gauge invariant phase different.

$$I_c = \cos\alpha + \cos\beta = 2\cos\frac{1}{2}(\alpha + \beta)\cos\frac{1}{2}(\alpha - \beta) \text{ Critical current}$$

$$\gamma = \emptyset_1 - \emptyset_2 - \frac{2\pi}{\emptyset_0}\int_1^2 Adl \tag{2.22}$$

The frequency of which given by:

$$f_j = \frac{u}{\emptyset_0} = u\frac{2e}{h} \tag{2.23}$$

The second Josephson equation:

$$\gamma^\cdot = \frac{2\pi}{\emptyset_0}u \tag{2.24}$$

2.9. Meissonier effect:

Meissonier and Ochsenfeld discovered in 1933 that a superconductor expelled the magnetic flux as the former cooled below T_c in an external magnetic field it behaved as a perfect diamagnetism. Such flux exclusion is also doing served if the superconductor first cooled below T_c and then placed in the magnetic field, since $B = 0$ inside the superconductor [10, 13].

$$B = \mu_0(H + M) = 0 \tag{2.25}$$

Where μ_0 the permeability of air and M the magnetization.

There for, the susceptibility given by:

$$x_M = \frac{M}{H} = -1 \tag{2.26}$$

That true for a perfect diamagnet.

$$\nabla \times E = -\frac{dB}{dt} \qquad \text{B= constant.} \tag{2.27}$$

Chapter Three

High temperature superconductivity

3.1. Introduction:

High temperature superconductors (HTS) are materials with much higher transition temperatures than already known superconductors. Whereas "ordinary" or metallic superconductors usually have transition temperature below 30k (-243.2c°), HTS have been observed with transition temperature as high as (38k (-135c°)) on the other hand, yield very direct information about the magnitude and the momentum dependence of the order parameter, as well as its evolution with temperature tunneling. Angle – resolved photoemission spectroscopy (ARPES) measurements experiments indicate that $d_{x^2-y^2}$ order parameter is the most plausible candidate to describe the superconducting state in these systems. The first high–T_C superconductor discovered in 1986 by IBM researchers Georg Bednorz and K-Alex Muller [14, 15].

3.2. The Chemistry structure of Superconductors:

The high-temperature superconductors (Perovskites) are a mixture of metal oxides, which display the mechanical and physical properties of ceramics. ($YBCO$) is a very common Type II superconductor. A key element to the behavior of these materials is the presence of planes containing copper and oxygen atoms chemically bonded to each other. The special nature of the copper-oxygen chemical bond permits materials to conduct electricity very well in some directions. Most ceramic materials considered good electrical insulators. $YBCO$ Compounds, also known as $1-2-3$ compounds, are very sensitive to oxygen content. They change from

semiconductors at $YBa\ Cu\ O\ 2\ 3\ 6.5$ to superconductors at $YBa\ Cu\ O\ 2\ 3\ 7$ without losing their crystalline structure, as in figure (3.1). The high sensitivity of superconductors to oxygen content is due to the apparent ease to which oxygen can move in and out of the molecular lattice. Using the standard valance charges for the metallic elements, one would expect a formula of $YBa\ Cu\ O$. However, 2 3 6.5 found that these superconductors usually have more oxygen atoms than predicted. According to the formula, $YBa\ Cu\ O$, the 2 3 7 metals are in a mole ratio of $1 - 2 - 3$ [7].

$YBaCuO$ is the first material found to be superconducting above liquid nitrogen $237c^0$ temperature. It exhibits a very interesting and complex relationship between its chemistry crystal structure and physical properties. In oxygen deficient $YBaCuO$, oxygen removed from the CuO chains. A 90 K 2 3 7x superconductor is obtained for $0 < x < 0.2$, a 60 K superconductor for $0.3 < x < 0.55$, and an antiferromagnetic semiconductor for $0.55 < x < 1.0$ [16].
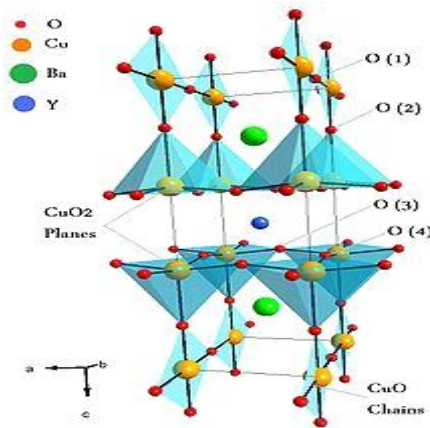

Figure (3.1) the crystal structure of $YBCO$

3.3. d-orbitals

For the d-orbital $L = 2$ and m can take values -2, -1, 0, +1 and +2. The orbital named as d_{xy}, d_{yz}, d_{xz}, $d_{x^2-y^2}$ and d_{z^2} as shown in figure (3.2). All the d_{xy}, d_{yz}, d_{xz} and $d_{x^2-y^2}$ orbitals have four lobes alternating in sign, opposing pairs being of the same sign. In the absence of the magnetic and electrical fields they are all equivalent in energy and are said to be fivefold degenerate. Three out of the five d-orbital, d_{xy}, d_{yz} and , d_{xz} have lobes symmetrically between the axial directions, namely, between x and y axes, y and z axes and x and z axes respectively. When the lobes of $d_{x^2-y^2}$ orbital lie along x and y-axes, while those of the d_{z^2} lie on the z-axis. Thus the d-orbital can be divided in to two groups; one group comprises the $d_{x^2-y^2}$ and the d_{z^2} orbitals which point along the axial directions, and the second group consists of the d_{xy}, d_{yz} and, d_{xz} orbitals which point along 45° to the axial directions. The energy of the orbital was increase in the order $s < p < d$ [16].
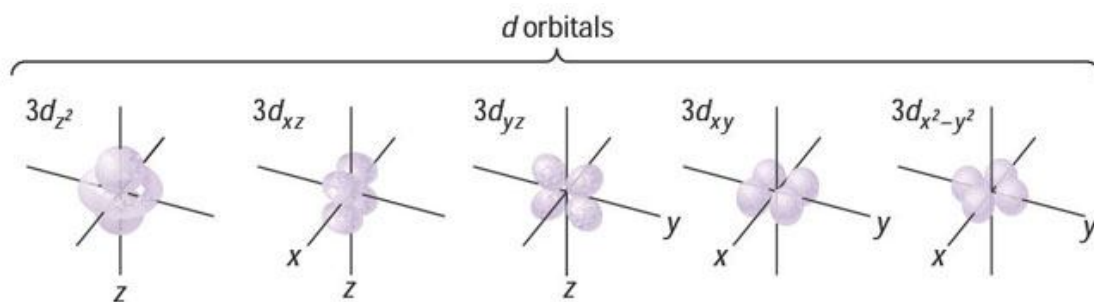

Figure (3.2) the shapes of the d-orbital

3.4. Hubbard Model and band structure:

The electronic configurations of several atoms occur at high temperature superconductors. The notation used is nl^N, where n is the principal quantum number, the orbital quantum number $l = 0$ for an s state, $l = 1$ for a p state, $l = 2$ for a d wave, and N is the number of electrons in each l state. A full l state contains $2(2l + 1)$ electrons. Correspond to 2,6,10 for s, p and d state, respectively. The cu^{2+} ion $(3d^9)$ may be looked upon as filled d–shell, $(3d^{10})$ plus one $3d$ hole, and in the cuprates, this hole is a $d_{x^2-y^2}$ orbital in the CuO_2 plane. The various s, p and d wavefunctions called orbitals have the unnormalized analytical forms, the orbitals $\emptyset(r - R)$ used in band structure calculations are normalized $\int \emptyset^*(r - R)\emptyset(r - R)d^3r$ for an atom located at position R. the overlap integral as

$$\delta(R - R^{'}) = \int \emptyset^*(r - R)\emptyset(r - R')d^3r \qquad (3.1)$$

Is a measure of the extent to which the orbitals of atom at positions R and $R^{'}$ overlap. The coulomb integral $u(R)$ equal;

$$u(R) = \int \emptyset^*(r - R)v_c(R)\emptyset(r - R')d^3r, \qquad (3.2)$$

Provides the coulomb repulsion energy associated with orbital $\emptyset(r - R)$ atom at position R. The Hamiltonian written in terms of creation $(a_\sigma^\dagger)$ and annihilation (a_σ) operators of spin σ associated with atoms at positions $R^{'}$ and R in the form:

$$H = -t \sum_{RR',\sigma} a_\sigma^\dagger(R) + a_\sigma(R') + \sum_{RR',\sigma} a_\sigma^\dagger(R') + a_\sigma(R)$$

$$-\mu \sum_{R,\sigma} a_\sigma^\dagger(R) + a_\sigma(R) + u \sum_R n + (R)n - (R) \qquad (3.3)$$

Where u is coulomb repulsion and the hopping amplitude t > 0 measure of the contribution from an electron hopping from one site to another. The chemical potential μ takes into account changes in the number of electrons and is zero if there is no doping. This Hamiltonian exhibits an electron-hole symmetry, which is of some importance because most high temperature superconductors are hole types with a close to half-full band [17].

3.5. Phase Diagrams:

Phase diagrams are critical research for many scientific disciplines including materials science, ceramics, engineering and Chemistry. These diagrams contain important information for the development of new materials, control of structure and composition of critical phases and improvement of properties of technologically important materials [8].

All copper oxides undergo several phase transitions as a function of oxygen content. In figure (3.3) we saw that at very low oxygen contents ($YBa_2Cu_3O_6$) and high temperatures, the material is a dielectric. At lower temperatures below a certain Neel temperature, the material becomes antiferromagnetic. The magnetic moments appear on the Cu atoms on the CuO_2 planes. Still at low temperatures, at higher oxygen contain, the material becomes metallic and superconductor. The critical temperature rises up to $92K$ for $YBa_2Cu_3O_6$. This knows "the optimal doping" [9].
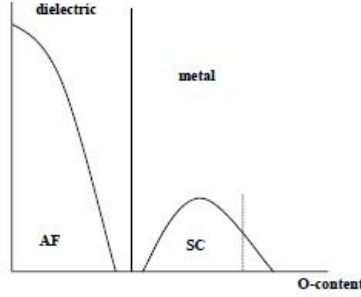
Figure (3.3) phase diagram for $(YBa_2Cu_3O_6)$

3.6. The pseudogap:

Gap symmetry used to explain the mechanism of high temperature superconductivity. One of the possible explanations of the pseudogap is superconducting fluctuations above the transition temperature. Superconducting fluctuations in their simplest form are due to small regions of normal material becoming superconducting by releasing some of their thermal energy to their vicinity. Since the superconducting region cannot be smaller than the size of a Cooper pair (ξ, the coherence length), the minimum required energy to create a superconducting fluctuation is proportional to ξ^2, the area of the region appropriate superconducting (2D fluctuations are considered). The coherence length of the cuprates is in turn very small, usually two orders of magnitude smaller than in the conventional superconductors. In addition, the transition temperature T_C is much higher in the cuprates, which makes fluctuations in the thermal energy larger [8, 18].
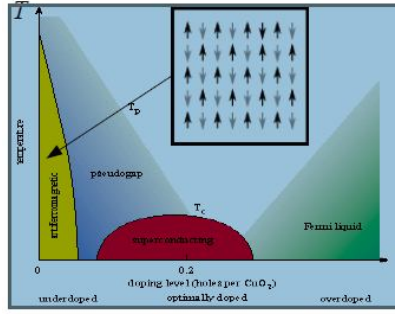
Figure (3.4) show the pseudogap and antiferomagnetic

The coherence length of the cuprates equal:

$$\xi_s = \frac{\hbar v_f}{\Delta_0} \tag{3.4}$$

Where v_f the velocity of the Cooper pairs at the Fermi surface.

$\Delta_0 = 1.76\, K_B T$ the gap energy.

The free energy for the high$-T_C$ superconductors given by

$$F_s = F_n + F_0^{tet} + F_0^{orth} + F_1^s + F_1^d + \frac{h^2}{8\pi} \tag{3.5}$$

Where F_n is the normal state free energy, F_0^{tet} and F_0^{orth} the lowest-order contribution for the free energy with tetragonal and orthorhombic symmetries. F_1^s, F_1^d the higher order tetragonal contribution involving s-wave and d-wave.

3.7. The tight binding approximation:

The tight binding approximation used to calculate the electron dispersion relation in periodic potentials. We consider a one-dimensional

crystal with a primitive cell that contains one atom and with lattice sites at positions $x_n = nL$ [19].

Where n is an integer and L the nearest neighbor atom spacing. $V(x - x_n)$ the potential of the n atom at position $x_n = nL$.

The time independent Schrodinger equation for an electron at position x as

$$\hat{H}\psi_{k_x}(x) = \left(\frac{-\hbar^2}{2m_0}\frac{d^2}{dx^2} + \sum_n V(x - x_n)\right)\psi_{k_x}(x) = E\psi_{k_x}(x) \qquad (3.6)$$

Where $\psi_{k_x}(x)$ Wave function that must satisfy the Bloch condition,

$$(x + L) = \psi_{k_x}(x)e^{ik_x L} \qquad (3.7)$$

k_x the Bloch wave vector.

We used delocalized Bloch functions $\psi_{k_x}(x) = U_{k_x}(x)e^{ik_x x}$ for which

$$U_{k_x}(x) = U_{k_x}(x + L) \qquad (3.8)$$

The Wannier functions $\phi(x)$ are localized around the lattice site x_n and are orthogonal for different lattice points so that;

$$\int \phi^*(x - x_m)\phi(x - x_n)dx = \delta_{mn} \qquad (3.9)$$

$$\psi_{k_x}(x) = \sum_n e^{ik_x x_n} \phi(x - x_n) \qquad (3.10)$$

The expectation value of electron energy is

$$E_{k_x} = \int \psi_{k_x}^*(x)\hat{H}\psi_{k_x}(x)dx +$$

$$\sum_{x_m}\sum_{x_n} e^{ik_x(x_n - x_m)} \int \phi_{k_x}^*(x - x_m)\hat{H}\phi_{k_x}(x - x_n)dx \qquad (3.11)$$

The first integral indicated for atom energy levels,

$$-E_0 = \int \psi_{k_x}^*(x)\hat{H}\psi_{k_x}(x)dx \tag{3.12}$$

Moreover, the second integral is the contribution from overlaps of nearest neighbors.

$$-t = \int \phi_{k_x}^*(x - x_m)\hat{H}\phi_{k_x}(x - x_n)dx \tag{3.13}$$

Where $x_m = x_n \pm L$, t the overlap integral with the sign convention.

$$E_{k_x} = -E_0 - t\left(e^{ik_xL} + e^{-ik_xL}\right) = -E_0 - 2t\cos(k_xL) \tag{3.14}$$

This cosine tight binding band for nearest neighbor interactions in one dimension has an energy bandwidth of $E_b = 4t$.

We assume $E_0 = 0$ that giving

$$E_{k_x} = -2t\cos(k_xL) \tag{3.15}$$

If one includes next neighbor interaction then there is an additional overlap integral t' involving sites

$$x_m = x_n \pm 2L$$

The energy dispersion gives by:

$$E_{k_x} = -2t\cos(k_xL) - 2t'\cos(2k_x L). \tag{3.16}$$

3.8. The Second Quantization for Bosons:

The Hamiltonian of system content N boson in volume V given by:

$$\hat{H} = \hat{T} + \hat{V} \tag{3.17}$$

Where $\hat{T}$ the kinetic energy operator in the form,

$$\hat{T} = -\frac{\hbar^2}{2m}\sum_{p=1}^{N}\nabla^2 p \tag{3.18}$$

For the second quantization, we rewrite the (3.18) in the form:

$$\hat{T} = \sum_k \frac{k^2}{2m}\hat{n_k} = \sum_k \frac{k^2}{2m}a_k^+ a_k \tag{3.19}$$

Where $\hbar=1$ the number operator $\hat{n_k} = a_k^+ a_k$ is creation and inhalation operators respectively. In addition, the potential energy operator is

$$\hat{V} = \frac{1}{2}\sum_{p=1}^{N}\sum_{s=1}^{N}V(|r_p - r_s| - \frac{1}{2}\sum_{s=1}^{N}v(0)) = \frac{1}{2}\iint \rho(r)^v(r-r')\rho(r')d^3rd^3 r' - \frac{1}{2}\int \rho(r)v(0)d^3r' \tag{3.20}$$

Where $r_p - r_s$ the distance between any interaction particle p, s and $\rho(r)$ is the density of particle in position $\vec{r}$ define as

$$\rho(r) = a^\dagger(r)a(r)$$

$$a^\dagger(r) = \frac{1}{\sqrt{v}}\sum_k a_k^\dagger e^{ik.r}$$

$$a(r) = \frac{1}{\sqrt{v}}\sum_k a_k e^{-ik.r} \tag{3.21}$$

Since we are using a representation plane wave states

$$\rho(r) = \frac{1}{V}\Sigma_{k,k'} a_k^\dagger a_{k'} e^{i(k-k').r} \tag{3.22}$$

We insert Fourier transform for the function $V(|r-r'|)$ to find

$$V(|r-r'|) = \Sigma_q v(q)e^{iq.(r-r')} \tag{3.23}$$

Then substitute equations (21.22.23) in equation (3.20) that give:

$$\hat{V} = \frac{1}{2v^2}\Sigma v(\vec{q})a_{k_1}^\dagger a_{k'_1} a_{k_2}^\dagger a_{k'_2} \iint e^{-i(k_1-k'_1).r} e^{i(k_2-k'_2).r} d^3r d^3r' - \frac{1}{2v}\Sigma_{k_1 k'.q} v(q)a_{k_1}^\dagger a_{k'_1} \int e^{i(k_2-k'_2).r} {}'d^3r' \tag{3.24}$$

Now remove some of summation over the momentum to give:

$$\hat{V} = \frac{1}{2}\sum_{k_1 k_2 q} v(q)a_{k_1}^\dagger a_{k_1-q} a_{k_2}^\dagger a_{k_2+q} - \frac{1}{2}\sum_{q k_1} v(q)\, a_{k_1}^\dagger a_{k_1}$$

$$= \frac{1}{2}\Sigma_{k_1,k'_{1-q}} v(q)\, a_{k_1}^\dagger a_{k_2}^\dagger a_{k_1-q} a_{k_2+q} + \frac{1}{2}\Sigma_{k_1,k_2,q} v(q)a_{k_1}^\dagger a_{k_2+q} - \frac{1}{2}\Sigma_{q,k_1} v(q)a_{k_1}^\dagger a_{k_1} \tag{3.25}$$

To used the commutation relation

$$[a_{k_1-q}, a_{k_2}^\dagger] = \delta_{k_2,k_1-q} \qquad [a_i, a_j^\dagger] = 0 \quad ; i \neq j$$

Then equation (3.25) reduced to:

$$\hat{V} = \frac{1}{2}\Sigma_{k_1,k'_{1-q}} v(q)\, a_{k_1}^\dagger a_{k_2}^\dagger a_{k_1-q} a_{k_2+q} \tag{3.26}$$

Finally, the Hamiltonian in second quantization from bosons becomes:

$$\hat{H} = \Sigma_k \frac{k^2}{2m} a_k^+ a_k + \frac{1}{2}\Sigma_{k_1,k'_{1-q}} v(q)\, a_{k_1}^\dagger a_{k_2}^\dagger a_{k_1-q} a_{k_2+q} \tag{3.27}$$

Chapter Four

d-wave Superconductivity

4.1. Introduction:

Cooper pairs in high-T_c superconductors determine by d-wave symmetry, especially $d_{x^2-y^2}$. This symmetry is internal and it appears in momentum space that means the wave function of the Cooper pair moving along the x-axis has + sign and that moving along y-axis has − sign.

In this chapter we described high-T_c compounds assume that a tetragonal lattice Symmetry, and use the symmetry properties to construct the form of the attractive interaction in the system [2, 15].

4.2. Model for d-wave superconductor:

In the BCS theory the isotropic electron-phonon interaction leads to an isotropic superconducting gap, this type of pairing symmetry called s-wave symmetry. The extended s-wave gap functions equal:

$$\Delta s^*(k) = \Delta_\circ (coskx + cosky), \qquad (4.1)$$

$$H = \sum_{k,\sigma}\left(\epsilon_k a_{k\sigma}^\dagger a_{k\sigma} + \Delta_k a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger\right) + h.c \qquad (٤.2)$$

Where the normal state dispersion given by a tight- binding Hamiltonian as

$$\epsilon_k = -2t\left(\cos k_x + \cos k_y\right) - t' \cos k_x \cos k_y - \mu \qquad (4.3)$$

Where t the contribution from hopping nearest neighbors, t' is the next nearest neighbors' interaction and μ the chemical potential.

In addition, the superconducting order parameter of $d_{x^2-y^2}$ symmetry equal,

$$\Delta_{d_{x^2-y^2}} = \frac{\Delta_0}{2}(\cos(k_x a) - \cos(k_y a)) \tag{4.4}$$

The $d_{x^2-y^2}$ wave pair field operator equal;

$$\hat{\Delta}^\dagger_{d_{x^2-y^2}} = \sum_k \Delta_{d_{x^2-y^2}}(k) a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow} \tag{4.5}$$

$$\hat{\Delta}^\dagger_{d_{x^2-y^2}} = \frac{\Delta_0}{2} \sum_l (a^\dagger_{l+x\uparrow} a^\dagger_{l\downarrow} - a^\dagger_{l+x\downarrow} a^\dagger_{l\uparrow}) - (a^\dagger_{l+y\uparrow} a^\dagger_{l\downarrow} - a^\dagger_{l+y\downarrow} a^\dagger_{l\uparrow}) +$$

$$(a^\dagger_{l-x\uparrow} a^\dagger_{l\downarrow} - a^\dagger_{l-x\downarrow} a^\dagger_{l\uparrow}) - (a^\dagger_{l-y\uparrow} a^\dagger_{l\downarrow} - a^\dagger_{l-y\downarrow} a^\dagger_{l\uparrow}) \tag{4.6}$$

As given, this Hamiltonian has nodal excitations, which are located along the $d_{x^2-y^2}$ symmetry axis in the $(\pm\pi, \pm\pi)$ directions. The nodes 'distance from $(\pm\pi/2, \pm\pi/2)$ controlled by the chemical potential μ. These quasi particles are Dirac fermions in the sense that they have conical dispersion [15].

The excitation energy is

$$E_k = \sqrt{\epsilon_k^2 + \Delta_k^2} \tag{4.7}$$

Return to Schrodinger's equation

$$\frac{R}{2} a_k \left(\frac{\hbar^2 k^2}{m_e} - E\right) = -\sum a_{k\prime} V_{kk\prime} \tag{4.8}$$

We define ϵ_k the energy above E_F, so

$$\epsilon = \left(\frac{\hbar^2 k^2}{m_e} - E_F\right) \tag{4.9}$$

ϵ the energy of electron pair; and E the energy below the Fermi energy.

$$\Delta = E_F - E \tag{4.10}$$

Where Δ is called the binding energy, given by

$$\Delta = \hbar\omega_D \exp\left(\frac{2\pi k_F}{m_e l V_0}\right) \tag{4.11}$$

Then the Schrodinger equation becomes:

$$\frac{R}{2}a_k(\epsilon + \Delta) = -\sum a_{k\prime}V_{kk\prime} \tag{4.12}$$

Moreover, at low energies $\epsilon_k \sim v_f k_1$ and $\Delta_k \sim v_\Delta k_2$, where k_1 and k_2 are displacements resulting from the normal state dispersion linear parallel to Fermi surface, and linear gap perpendicular to the Fermi surface, with slopes v_f and Δ_k . For μ on the order of t or smaller, the velocity given as

$$\frac{v_f}{v_\Delta} \approx \frac{\sqrt[4]{t^2} - \frac{\mu}{t}t'^2}{\Delta_0} \tag{4.13}$$

Then, as perturbations turned on, the locations of the nodes evolves in k-space, although the stability of the nodes preserved for non-nesting perturbations that preserve the composite symmetry of lattice [17].

4.3. The wave function of d-orbitals:

The wave function of d-orbitals represented by the separated two radial wave function and angular wave function in the form:

$$\psi_{3dx^2-y^2} = R_{3d}Y_{3dx^2-y^2} \tag{4.14}$$

Where $\quad R_{3d} = \left(1/\sqrt[9]{30}\right)\rho^2 Z^{3/2}e^{-\rho/2} \tag{4.15}$

$$\rho = \frac{2Zr}{n}$$

n is the principle quantum number, r radius expressed in atomic units.

Z is effective nuclear charge for orbital in the atom.

The angular wave function as

$$Y_{3dx^2-y^2} = \sqrt{\frac{15}{4}} \frac{(x^2-y^2)}{r^2} \left(\frac{1}{4\pi}\right)^{1/2} \tag{4.16}$$

The electron Hamiltonian represented as a sum of one- and two-electron terms:

$$H = H_0 + H' \tag{4.17}$$

$$H = \sum_{i=1}^{N} \epsilon(x_i) - \frac{1}{2}\sum_{i \neq j}^{N} \sum_{j}^{N} \upsilon(x_i, x_j) \tag{4.18}$$

Now rewrite the Hamiltonian for the electrons in terms of electron creation and destruction operators as

$$H_0 = \sum_{i=1}^{N} \epsilon(x_i) = \sum_{i,j} \langle \phi_i | \epsilon | \phi_j \rangle a_i^\dagger a_j = \sum_{i,j} \epsilon_{ij} a_i^\dagger a_j \tag{4.19}$$

$$\epsilon_{ij} = \langle \phi_i | \epsilon | \phi_j \rangle = \int \phi_i^* (x)\epsilon(x)\phi_j(x)dx \tag{4.20}$$

The operator for the electron-electron interaction H' acquires at the form:

$$H' = \frac{1}{2}\sum_{i,j,k,l} \langle \phi_i \phi_j | \upsilon | \phi_k \phi_l \rangle a_i^\dagger a_j^\dagger a_l a_k \tag{4.21}$$

Where $a_l a_k$ The destruction operators and ϕ_i, ϕ_j the spin-orbital of electrons.

$$\langle \phi_i \phi_j | \upsilon | \phi_k \phi_l \rangle = \iint \phi_i^*(x_1) \phi_j^*(x_2)\upsilon(x_1, x_2)\phi_k(x_1)\phi_l(x_2)dx_1 dx_2 \tag{4.22}$$

Finally the Hamiltonian written as

$$H = \sum_{i,j=1}^{N} \langle \phi_i | \epsilon | \phi_j \rangle a_i^\dagger a_j + \frac{1}{2}\sum_{i,j,k,l} \langle \phi_i \phi_j | \upsilon | \phi_k \phi_l \rangle a_i^\dagger a_j^\dagger a_l a_k \tag{4.23}$$

This Hamiltonian similar to Hamiltonian in equation (3.27) those described the kinetic energy and potential energy for cooper pair.

4.4. Evidence of d-wave pairing:

The evidence for d-wave superconductivity in the cuprates has obtained from experiments sensitive to changes in the sign of the gap function. Line nodes are a common feature of unconventional gap function symmetry, such as extended s-wave (with nodes along ($|k_x| = |k_y - \pi|$)), d-wave ($|k_x| = |k_y|$), and d_{xy}-wave ($k_x = 0, k_y = 0$). In conventional superconductors, the number of excitations at low temperatures is $e^{-\Delta/k_B T}$ due to the presence of a non-zero gap. The low temperature behavior of the penetration depth in the cuprates suggests a gap with line nodes [20].

All experiments indicate that the phase of the d-wave order parameter differs by π between the [100] and [010] directions of the CuO_2 plane because the lobes of the gap function aligned with the crystal axes. The modulation of the critical current has measured for the cuprate superconductor. If the cuprates were an s-wave superconductor, the supercurrent should be a maximum in the absence of an applied field H. If the cuprate were a d-wave superconductor, appositive lobe would face the other; the resulting destructive interference should yield zero supercurrent when $H = 0$, but a maximum current for $H = \phi_0/2 = \pi$.

4.5. Conclusion:

The pairing of the electrons around the Fermi surface creates a range of energies, which depleted of single electron excitations, this called, superconducting gap. Equation (4.10), high- T_C superconductors are magnetic systems due to the Coulomb interaction; there is a strong Coulomb repulsion between electrons, this Coulomb repulsion prevents pairing of the Cooper pairs on the same lattice site. The pairing of the electrons occurs at near-neighbor lattice site this called *d*-wave pairing, where the pairing state has a node (zero) at the origin. The weak isotope effects observed for most cuprates contrast with conventional superconductors that well described by BCS theory.

In this research, we used quantum mechanics to describe the energy gap of the materials, which a characterized by superconducting at high temperatures described by $d_{x^2-y^2}$ symmetry, equation (4.4) comparing with the energy gap in BCS theory and found that Cooper pairs can be described as boson.

4.6. Recommendation:

We recommended to further study to:

•More researchers to study the mechanism of the internal structure of Cooper pair to explain the phenomena of high T_c cuprates.

• develop the model of d-wave that describes the superconducting compounds at high temperature.

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