

Using the tight binding approximation in deriving the quantum critical temperature superconductivity equation

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ABSTRACT

Superconductivity is one of the most important phenomena in solid state physics. Its theoretical framework at low critical temperature T_c is based on Bardeen, Cooper and Schrieffer theory (BCS). But at high T_c above 135, this theory suffers from some setbacks. It cannot explain how the resistivity abruptly drops to zero below T_c , besides the explanation of the so called pseudo gap, isotope and pressure effect, in addition to the phase transition from insulating to superconductivity state. The models proposed to cure this drawback are mainly based on Hubbard model which has a mathematical complex framework. In this work a model based on quantum mechanics besides generalized special relativity and plasma physics. It is utilized to get new modified Schrödinger equation sensitive to temperature. An expression for quantum resistance is also obtained which shows existence of critical temperature beyond which the resistance drops to zero. It gives an expression which shows the relation between the energy gap and T_c . These expressions are mathematically simple and are in conformity with experimental results.

Keywords: Superconductivity; High Critical Temperature; Tight Binding Approximation

1. INTRODUCTION

Superconductivity (SC) was discovered in 1911 in the Leiden laboratory of Kamerlingh Onnes when a so called “blue boy” (local high school student recruited for the tedious job of monitoring experiments) noticed that the

resistivity of Hg metal vanished abruptly at about 4 K. Although phenomenological models with predictive power were developed in the 30's and 40's of the last century [1], F and H London developed the successful phenomenological approach in 1935 describing the behavior of superconductors in the external magnetic field. Ogg Jr. proposed a root to high-temperature superconductivity (HTSC) introducing electron pairs in 1946 and Ginzburg and Landau proposed the phenomenological theory of the superconducting phase transition in 1950 providing a comprehensive understanding of the electromagnetic properties below T_c [2]. The microscopic mechanism underlying superconductivity was not discovered until 1957 by Bardeen Cooper and Schrieffer (BCS) [1]. Superconductors have been studied intensively for their fundamental interest and for the promise of technological applications which would be possible if a material which superconducts at room temperature was discovered. Until 1986, critical temperatures (T_c 's) at which resistance disappears were always less than about 23 K.

In 1986, Bednorz and Mueller published a paper, subsequently recognized with the 1987 Nobel Prize, for the discovery of a new class of materials called (HTSC) which currently include members with T_c 's of about 135 K or more. Enormous numbers of studies have been carried out to clarify the mechanism of the high temperature superconductivity (HTSC) beyond the conventional BCS theory **Figure 1**.

One of the important HTSC is the cuprate compounds. The cuprate systems show not only high temperature superconductivity but also show various unusual behaviors when doped with holes where it is converted from an insulator to a superconductor [1]. The transition-metal oxides have been extensively investigated in recent years as materials that can be converted to superconductors. Understanding the nature of superconductors has been

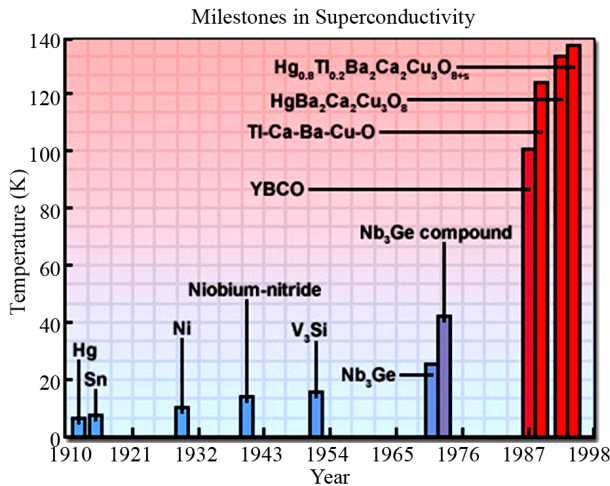


Figure 1. History of superconductivity.

the most challenging issue in condensed matter physics due to the difficulties inherent in the many-body interactions.

Although BCS theory explains several superconductors phenomena specially at low critical temperature T_c , but there are many setbacks associated with Bardeen, Cooper and Schrieffer BCS theory for high critical temperature $T_c \geq 135$, which was observed in some compounds specially CuO and Fe compounds.

There are many problems need to be solved. First of all, one observes that, till now, there is no well established theoretical expression in most celebrated SC models which shows how the resistance drops abruptly to zero below the critical temperature. The existence of an energy gap well above T_c with pressure and the substitution of O^{16} by its isotope O^{18} affecting T_c also need to be explained by a simple model also.

The aim of this work is to construct quantum mechanical model based on plasma equation to construct a quantum model which explains why the resistance vanishes below critical temperature. It also aimed to find a useful expression for the energy gap. These contribution are exhibited in Sections (5) and (6). Section (2) is devoted for the theoretical plasma equation.

2. PLASMA EQUATION

According to plasma equation, a fluid of particles of mass m , number density n , velocity v , force F and pressure P is given by

$$mn \left[\frac{\partial v}{\partial t} + v \cdot \nabla v \right] = F - \nabla P \tag{1}$$

If F is a field force then

$$F = -n \nabla V$$

Where V is the potential of one particle. In one dimension

$$mn \left[\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} \right] = -n \nabla V - \nabla P = -n \frac{dV}{dx} - \frac{dP}{dx}$$

$$dv = \frac{\partial v}{\partial t} dt + \frac{\partial v}{\partial x} dx$$

$$\frac{dv}{dt} = \frac{\partial v}{\partial t} + \frac{\partial v}{\partial x} \frac{dx}{dt} = \frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} \tag{2}$$

Thus according to Equation (1), in one dimension

$$mn \frac{dv}{dt} = -n \frac{dv}{dx} - \frac{dp}{dx} \tag{2'}$$

3. SCHRÖDINGER TEMPERATURE DEPENDENT EQUATION

Schrodinger equation can be derived by using new expression of energy obtained from the plasma equation to do this one can use (2) to get

$$mn \frac{dv}{dx} \frac{dx}{dt} = -n \frac{dV}{dx} - \frac{dP}{dx}$$

Multiplying both sides by dx and integrating yields

$$mn \int v dv = -n \int dV - \int dP$$

Considering the pressure to be $p = \gamma nkT$ in general, thus

$$mn \frac{v^2}{2} = -nV - P = -nV - \gamma nkT$$

Hence

$$m \frac{v^2}{2} + V + \gamma kT = const$$

This constant conserved quantity looks like the ordinary energy beside the ordinary thermal energy term γkT .

$$E = \frac{p^2}{2m} + V + \gamma kT \tag{3}$$

To find Schrödinger equation for it, consider the ordinary wave function

$$\psi = A e^{i\hbar(px - Et)}$$

Differentiating both sides by t and x yields

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E \psi \Rightarrow i\hbar \frac{\partial \psi}{\partial t} = E \psi$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2} \psi \Rightarrow -\hbar^2 \nabla^2 \psi = p^2 \psi \tag{4}$$

Multiplying both sides of Equation (3) by ψ yields

$$E \psi = \frac{p^2}{2m} \psi + V \psi + \gamma kT \psi$$

Substituting Equation (4), one gets

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi + \gamma kT\psi$$

This equation represents Schrödinger equation when thermal motion is considered. The solution for time free potential can be

$$\psi = e^{-i/h(Et)} u \Rightarrow \frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E\psi$$

$$E\psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi + \gamma kT\psi$$

The time independent Schrödinger equation thus takes the form

$$Eu = -\frac{\hbar^2}{2m} \nabla^2 u + Vu + \gamma kTu \tag{5}$$

For constant potential, the solution can be

$$u = e^{ikx}, \quad V = V_o$$

Inserting this solution in Equation (5) yields

$$Eu = \frac{\hbar^2 k^2}{2m} u + V_o u + \gamma kTu$$

$$E = \frac{\hbar^2 k^2}{2m} + V_o + \gamma kT$$

If one set the kinetic term to be $E_o = \frac{\hbar^2 k^2}{2m}$, one can thus write the energy in the form

$$E = E_o + V_o + \gamma kT \tag{6}$$

This quantum energy expression involves a thermal term beside kinetic and potential term.

4. QUANTUM RESISTANCE

The resistance, z , per unit length ($L = 1$) per unit area ($A = 1$) can be found from the ordinary definition of, z . The resistance z is defined to be the ratio of the potential, u , to the current per unit area, J , i.e.

$$z = \frac{u}{I} = \frac{u}{JA} = \frac{u}{J} = \frac{u}{nev} = \frac{mu}{nep} \tag{7}$$

With n and e standing for the free hole or electron density and charge respectively, while p represents the momentum of electron of mass m , where $P = mv$.

This resistance (it actually stands for resistivity) can be found by using the laws of quantum mechanics for a free charge which are responsible for generating the electric current, where the wave function takes the form

$$\psi = Ae^{ikx} \tag{8}$$

This selection of ψ comes from the fact that the resistance property comes from the motion of the free

charges. The potential u is related to the Hamiltonian H through the relation

$$H = eu$$

Thus for freely moving charge one gets:

$$\hat{H} = eu = \frac{1}{2}mv^2 = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2$$

In view of Equation (8) and according to the correspondence principle V takes the form

$$u = \frac{\langle \hat{H} \rangle}{e} = \frac{\int \bar{\psi} \hat{H} \psi dx}{e} = \frac{\int \bar{\psi} \hat{p}^2 \psi dx}{2me} \tag{9}$$

$$= \frac{\hbar^2 k^2}{2me} \int \bar{\psi} \psi dx = \frac{\hbar^2 k^2}{2me}$$

While P becomes

$$p = \langle \hat{p} \rangle = \int \bar{\psi} \hat{p} \psi dx = \hbar k \int \bar{\psi} \psi dx = \hbar k \tag{10}$$

Thus inserting Equations (9), (10) in (7) one obtains

$$Z = \frac{m\hbar^2 k^2}{2me^2 \hbar kn} = \frac{\hbar k}{2e^2 n} = \left(\frac{h}{2\pi} \right) \left(\frac{2\pi}{\lambda} \right) \frac{1}{2e^2 n}$$

$$z = \frac{h}{2\lambda e^2 n} = \frac{hf}{2f\lambda e^2 n} = \frac{hf}{2e^2 nv} = \frac{hf\sqrt{\mu\epsilon}}{2e^2 n} = \frac{\hbar\omega\sqrt{\mu\epsilon}}{2e^2 n} \tag{11}$$

where the expression $f\lambda$ for velocity is found by assuming charges to be waves, then following the electromagnetic theory (EMT), the speed of the waves is affected by electric permittivity ϵ and magnetic permeability through the relation

$$v = \lambda f = \frac{1}{\sqrt{\mu\epsilon}} \tag{12}$$

where the effect of medium changes the wave length, λ , while the frequency, f , is unchanged. Thus assuming the charge density, n , to be constant, the only change of, Z , can be caused by μ and ϵ .

It is also important to note that, in superconductors, the current can flow without the aid of deriving potential u . the role of u is confined only in enabling electrons to gain kinetic energy through the relations

$$eu = \frac{1}{2}mv^2 = k \tag{13}$$

where this potential can be applied between any two arbitrary points in the superconductors then remove it. The role of resistive force is neglected here as done in deriving London equations.

The expression for Z can also be found by inserting Equation (13) in to get

$$Z = \frac{u}{J} = \frac{u}{nev} = \frac{mv^2}{2ne^2 v} = \frac{mv}{2ne^2} = \frac{p}{2ne^2} = \frac{h}{2\lambda ne^2}$$

$$Z = \frac{hf}{2\lambda fe^2 n} = \frac{hf}{2e^2 nv} = \frac{hf\sqrt{\mu\epsilon}}{2e^2 n} = \frac{\hbar\omega\sqrt{\mu\epsilon_o}(1+\chi)}{2e^2 n} \tag{14}$$

It is important to note that this quantum resistance expression resembles the ones found by Tsui [3] where one uses De Broglie hypothesis [4], i.e. $p = h/\lambda$.

5. CALCULATION HTSC BY ELECTRIC SUSCEPTIBILITY

Consider holes in a conductor having resistive force F_r , magnetic force F_m and pressure force F_p , beside the electric force F_e , the equation motion then becomes [3]:

$$F = F_r + F_m + F_e - F_p$$

where

$$F_p = -\nabla P, F_r = -\frac{mv}{\tau}, F_m = Bev, F_e = eE = eE_0 e^{i\omega t}$$

P, x, m, v, τ, B, e and E stands for the pressure, displacement, mass, velocity, relaxation time, magnetic flux density, electron charge and electric field intensity respectively. Thus the equation of motion takes the form

$$m\ddot{x} = -\frac{mv}{\tau} + Bev + eE - \nabla P \tag{15}$$

The solution of this equation can be suggested to be:

$$\begin{aligned} x &= x_0 e^{i\omega t} \\ v &= v_0 e^{i\omega t} \\ E &= E_0 e^{i\omega t} \end{aligned} \tag{16}$$

Inserting (16) in (15) yields

$$\begin{aligned} -m\omega^2 x &= \left(-\frac{mv_0}{E_0\tau} + \frac{Bev_0}{E_0} - \frac{kT\nabla n}{E_0} + e \right) E \tag{17} \\ x &= \frac{\left(\frac{mv_0}{E_0\tau} - \frac{Bev_0}{E_0} + \frac{kT\nabla n}{E_0} - e \right) E}{m\omega^2} \end{aligned}$$

This expression of x can be utilized in the formula which relates the electric polarization vector P to the susceptibility χ on one hand and to the number of atoms N via the following relation

$$P = \epsilon_0 \chi E = +eNx \tag{18}$$

Motivated by the important role of holes in HTSC, displacement can be assumed to result from the motion of holes or positive nuclear charges, thus inserting Equation (17) in (18) yields

$$\begin{aligned} \epsilon_0 \chi E &= eN \frac{\left(\frac{mv_0}{E_0\tau} - \frac{Bev_0}{E_0} + \frac{kT\nabla n}{E_0} - e \right) E}{m\omega^2} \\ \chi &= \frac{eN}{m\omega^2 \epsilon_0 E_0} \left(\frac{mv_0}{\tau} - Bev_0 + kT\nabla n - eE_0 \right) \end{aligned} \tag{19}$$

The electric flux density assumes the following relation

$$D = \epsilon E = \epsilon_0 E + \chi \epsilon_0 E = \epsilon_0 (1 + \chi) E = P + \epsilon_0 E$$

The electric permittivity is given by

$$\epsilon = \epsilon_0 (1 + \chi) \tag{20}$$

The electric permittivity is thus given according to Equation (20) to be

$$\begin{aligned} \epsilon &= \epsilon_0 (1 + \chi) \\ &= \epsilon_0 \left[1 + \frac{eN}{m\omega^2 E_0} \left(\frac{mv_0}{\tau} - Bev_0 + kT\nabla n - eE_0 \right) \right] \end{aligned} \tag{21}$$

The resistance Z can be found by inserting (21) in (14) to get:

$$m\omega^2 \epsilon_0 E_0 + eN \left(kT\nabla n + \frac{mv_0}{\tau} - Bev_0 - eE_0 \right) < 0$$

$$kT\nabla n < +Bev_0 + eE_0 - \frac{m\omega^2 \epsilon_0 E_0}{eN} - \frac{mv_0}{\tau}$$

$$T < +\frac{Bev_0}{k\nabla n} + \frac{(e - m\omega^2 \epsilon_0) E_0}{eNk\nabla n} - \frac{mv_0}{\tau k\nabla n}$$

Thus the critical temperature is given by

$$T_c = \frac{(Be\tau - m)v_0}{\tau k\nabla n} + \frac{(e - m\omega^2 \epsilon_0) E_0}{eNk\nabla n} \tag{23}$$

If the internal field B results from N_0 atoms each having a verge flux density μB then: [5].

$$B = \mu_B N_0 \tag{24}$$

Therefore T_c can take the form

$$T_c = \frac{(\mu_B N_0 e\tau - m)v_0}{\tau k\nabla n} + \frac{(e - m\omega^2 \epsilon_0) E_0}{eNk\nabla n} \tag{25}$$

6. TIGHT BINDING CRITICAL TEMPERATURE AND ENERGY GAP

In tight binding model [5] the energy of electrons in

$$\begin{aligned} z &= \frac{\hbar\omega}{2ne^2} \sqrt{\mu\epsilon_0 \sqrt{1 + \frac{eN}{m\omega^2 \epsilon_0 E_0} \left(kT\nabla n + \frac{mv_0}{\tau} - Bev_0 - eE_0 \right)}} \tag{22} \\ z &= \frac{\hbar\omega}{2ne^2} \sqrt{\mu\epsilon_0 \sqrt{\frac{m\omega^2 \epsilon_0 E_0 + eN \left(kT\nabla n + \frac{mv_0}{\tau} - Bev_0 - eE_0 \right)}{m\omega^2 \epsilon_0 E_0}}} \end{aligned}$$

the crystal is given by

$$\varepsilon = \varepsilon_0 + \alpha_1 + 2\gamma \cos ka \tag{26}$$

where ε_0 is the energy in the absence of crystal field, while the other terms describe the effect of the crystal field. The energy ε_0 can split into two terms the kinetic part which can describe the thermal motion in the form $\frac{f_0}{2}kT$ beside the potential term $-V_0$ for attractive force or bounded particle.

Thus one can write

$$\varepsilon_0 = \frac{\hbar^2 k_o^2}{2m} + \frac{f_0}{2}kT - V_0 \tag{27}$$

$$E = \frac{\hbar^2 k_o^2}{2m} + \gamma kT + V$$

$$\varepsilon_0 = \frac{f_0}{2}kT - V_0 - \alpha_o$$

$$\alpha_o = \frac{\hbar^2 k^2}{2m}$$

f_0 represents the degrees of freedom.

The terms describing the effect of the crystal force are

$$\begin{aligned} \alpha_1 &= \langle \phi_m | \hat{H}_{cry} | \phi_m \rangle \\ \gamma &= \langle \phi_j | \hat{H}_{cry} | \phi_m \rangle \\ \alpha &= \alpha_o + \alpha_1 \end{aligned} \tag{28}$$

In view of Equations (26) and (27)

$$\varepsilon = \frac{f_0}{2}kT - V_0 + \alpha + 2\gamma \cos ka \tag{29}$$

Here H_{cry} stands for the crystal force Hamiltonian part, while ϕ_m and ϕ_j are the states of particles located at the site m and j respectively.

The superconductor is characterized by the existence of energy gap. This gap can be under stood here in two ways. If the electrons or holes are not free. This requires E to negative. Thus Equations (27) and (26) needs

$$\varepsilon = \frac{f_0}{2}kT - V_0 + \alpha + 2\gamma \cos ka < 0 \tag{30}$$

Or the max value of ε where $\cos ka = -1$ is less than zero, i.e.

$$\varepsilon_{max} = \frac{f_0}{2}kT - V_0 + \alpha + 2\gamma \cos ka < 0 \tag{31}$$

$$\frac{f_0}{2}kT \leq V_0 - \alpha + 2\gamma$$

For constant attractive crystal force

$$H_{cry} = -V_{cry}$$

$$\alpha_1 = \langle \phi_m | H_{cry} | \phi_m \rangle = -\langle \phi_m | V_{cry} | \phi_m \rangle = -V_{cry} \delta_{mm}$$

$$\gamma = \langle \phi_j | -V_{cry} | \phi_m \rangle = -V_{cry} \langle \phi_j | \phi_m \rangle = -V_{cry} \delta_{jm=0} \tag{32}$$

Thus

$$\frac{f_0}{2}kT \leq V_0 - \alpha$$

Thus the critical temperature is given by

$$\frac{f_0}{2}kT_c = V_0 - \alpha \tag{33}$$

Substituted Equation (33) beside Equation (32) in Equation (30) one gets

$$\varepsilon = \frac{f_0}{2}kT - \frac{f_0}{2}kT_c \tag{34}$$

The energy gap Δ s equal to the difference between zero energy in conduction band and the negative energy in the valence band. Thus

$$\Delta = 0 - \varepsilon = \frac{f_0}{2}kT_c - \frac{f_0}{2}kT$$

Since this relation holds for $T < T_c$ one can neglect T since it is small to get

$$\Delta = \frac{f_0}{2}kT_c$$

Equation (30) can also be utilized to get the forbidden energy states which characterizes superconductors, where

$$\cos ka = \frac{\varepsilon - \frac{f_0}{2}kT + V_0 - \alpha}{2\gamma}$$

The energy is forbidden when $\cos ka \geq 1$

$$\frac{\varepsilon - \frac{f_0}{2}kT + V_0 - \alpha}{2\gamma} \geq 1$$

$$\varepsilon - \frac{f_0}{2}kT + V_0 - \alpha \geq 2\gamma$$

$$\frac{f_0}{2}kT + \alpha - \varepsilon - V_0 \leq -2\gamma$$

$$\frac{f_0}{2}kT \leq \varepsilon + V_0 - 2\gamma - \alpha$$

Thus the critical temperature

$$\frac{f_0}{2}kT_c = \varepsilon + V_0 - 2\gamma - \alpha \tag{35}$$

The forbidden energy is thus related to the critical temperature through the relation

$$\varepsilon = \frac{f_0}{2}kT_c - V_0 + 2\gamma + \alpha \tag{36}$$

If the particle has a 4—degree of freedom, 3—translational and one vibration.

$$\varepsilon = 2kT_c - V_o + 2\gamma + \alpha \quad (37)$$

In view of Equations (32) and (28), since Plank constant is very small and for very small crystal field and for bound force $\varepsilon \approx 2kT_c$, since the energy gap Δ is the difference between bound valence energy E , and minimum free conduction electron energy zero. Thus

$$\Delta = E - 0 = 2kT_c \quad (38)$$

Which shows linear relation between Δ and T_c , thus it resembles the empirical relations. Where the energy gap is found to be $\Delta \sim 1.75kT_c$ [6].

7. DISCUSSION

This model predicts that Schrödinger equation can be derived by using a new expression of energy obtained from the plasma equation. This expression includes thermal energy beside kinetic and potential energy according to Equation (6) It is very striking to note that this expression resembles the expression of the thermodynamic internal energy. A useful quantum expression for resistivity is also obtained in Equation (11) this expression resembles those obtained by Aharonove, Bohm and Berry as pointed out at the end of section 4. The model predicts that the resistivity of low and high T_c superconductors it drop abruptly when $Z_1 = \text{real} = \text{zero}$ according to Equation (8). It also finds the critical temperature T_c beyond which the resistivity vanish according to Equations (23) and (24). A useful expression for the energy gap which is dependent on T_c is also obtained. This expression is in agreement with the empirical relation.

8. CONCLUSIONS

The plasma equation is utilized to derive new energy expression in which thermal energy is added to the ordi-

nary kinetic and potential energy. This quantum equation which is temperature dependent within the framework of this equation uses tight binding approximation besides the quantum impedance expression, and it is very easy to explain why resistance vanishes below a certain critical temperature and why the empirical relation between the energy gap and the critical temperature is linear.

This raises a hope that Schrodinger quantum temperature dependent model can be utilized, if a frictional effect can be incorporated in it, to construct a general theoretical frame work capable of describing Schrodinger phenomena. The result obtained indicates that the quantum plasma model can improve the theoretical model to explain some of the phenomena associated with the HTSC. Strictly speaking it can explain why the resistance drops abruptly below T_c , besides explaining some important effects like the relation between energy gap and critical temperature.

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