ปรากฏการณ์ไอโซโทปในตัวนำยวดยิ่งอุณหภูมิสูง

นายพงษ์แก้ว อุดมสมุทรหิรัญ

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรดุษฎีบัณฑิต
สาขาวิชาฟิสิกส์
มหาวิทยาลัยเทคโนโลยีสุรนารี
ปีการศึกษา 2544

ISBN 974-533-016-7

THE ISOTOPE EFFECT IN HIGH-T_c SUPERCONDUCTOR

Mr. Pongkaew Udomsamuthirun

A Thesis Submitted in Partial Fulfillment of Requirements

for the Degree of Doctoral of Science in Physics

Suranaree University of Technology

Academic Year 2001

ISBN 974-533-016-7

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Suranaree University of Technology Council has approved this thesis submitted in partial fulfillment of the requirements for a Doctoral Degree.

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....

(Assoc.Prof.Dr. Prasart Suebka)

Chairman

....

(Prof.Dr. Suthat Yoksan)

Thesis Adviser

....

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พงษ์แก้ว อุดมสมุทรหิรัญ : ปรากฏการณ์ไอโซโทปในตัวนำยวดยิ่งอุณหภูมิสูง (THE ISOTOPE EFFECT IN HIGH-T_c SUPERCONDUCTOR) อ.ที่ปรึกษา : ศ.ดร.สุทัศน์ ยกส้าน, 114 หน้า, ISBN 974-533-016-7

จุดมุ่งหมายของวิทยานิพนธ์นี้คือ การอธิบายปรากฏการณ์ไอโซโทปที่ไม่ปรกติในตัวนำยวดยิ่งอุณหภูมิสูง โดยพิจารณาอิทธิพลของช่องว่างเทียม ความหนาแน่นสถานะ อันตรกิริยาที่ใช้โฟนอนและอันตรกิริยาที่ใช้อิเล็กตรอน ในเงื่อนไขของอันตรกิริยาแบบอ่อน ได้ผลการคำนวณสมการแบบแม่นตรงของเลขชี้กำลังไอโซโทป α ในสมมาตรของการจัดคู่ของคลื่น s และ d โดยใช้ความหนาแน่นสถานะต่างๆกัน เช่น แบบคงตัว แบบวานโฮฟ และแบบยกกำลัง พบว่าค่าของ α สอดคล้องกับข้อมูลจากการทดลองโดยเฉพาะสูตรของ α ในสมมาตรแบบคลื่น d สอดคล้องกับผลการทดลองมากกว่าแบบคลื่น s

สาขาวิชาฟิสิกส์ ลายมือชื่อนักศึกษา________________________

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PONGKAEW UDOMSAMUTHIRUN : THE ISOTOPE EFFECT IN HIGH-T_c SUPERCONDUCTOR THESIS ADVISER : PROF.SUTHAT YOKSAN, Ph.D. 114 PP. ISBN 974-533-016-7

The purpose of this thesis is to explain the unusual isotope effect of high-T_c superconductor by considering the influence of the pseudogap, the density of states, the phononic and the electronic interactions in the weak-coupling limit. Exact analytical expressions for the isotope exponent (α) with s-wave and d-wave pairing symmetry are derived. By using the constant, Van Hove singularity and power law density of states cases we find that our formula for α fits well with the experimental data, especially in case of the d-wave pairing symmetry.

สาขาวิชาฟิสิกส์ ลายมือชื่อนักศึกษา______________________

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ACKNOWLEDGMENTS

The author wishes to express his appreciation to his adviser, Prof.Dr. Suthat Yoksan for his advice, guidance and encouragement given throughout the course of investigation. He would also like to thank the thesis committee for their reading and criticizing the manuscript.

Partial financial supports by the Thailand Research Fund and the Royal Golden Jubilee scholarship(RGJ) are gratefully acknowledged.

Finally, he would like to thank the extraordinary help and love of his parents, wife, and son given to him in the past, present, and future.

Pongkaew Udomsamuthirun

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CHAPTER I

INTRODUCTION

Basic Properties of Superconductors

Heike Kammerling Onnes was able to liquefy helium in 1908, the field of low-temperature physics started. Three years later, he reported another remarkable discovery. At 4.19 K, the resistance of mercury (Hg) dropped abruptly to zero. Thus, T_c = 4.19 K for Hg, and he found similar transitions in lead and tin and he called this new the state of matter the "superconducting state"(Kamerling Onnes, 1911).

Superconductivity is fairly common place among nonmagnetic metals. Of all the elements, Nb has the highest transition temperature (T_c=9.25 K). Table(1.1) lists T_c values for elements and a few of the hundreds of compounds that have been reported (Burns,1992).

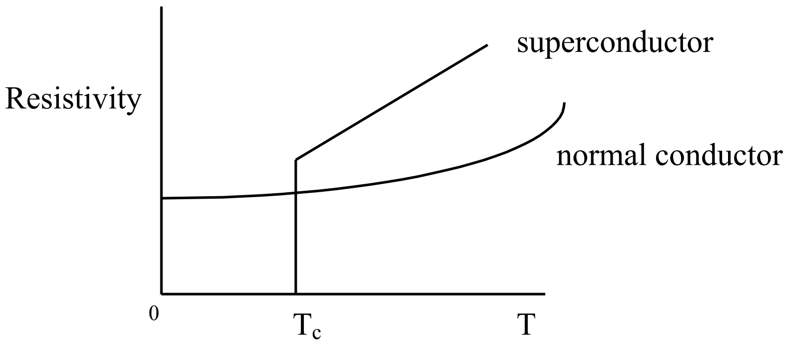
Element	T_c(K)	Compound	T_c(K)
Nb	9.25	Nb_3Ge	23.2
Pb	7.20	Nb_3Ga	20.3
V	5.40	Nb_3Au	10.8
Ta	4.47	V_3Si	17.1
Hg(α)	4.15	NbN	17.3
Hg(β)	3.95	MoC	14.3
Lu	0.10	UBe_{13}	0.85
Be	0.026	UPt_3	0.54

Table(1.1) Values of T_c for the elements and compounds that are superconducting at atmospheric pressure (Burns,1992).

In this section, we will show the experimental facts that has been observed in the matter in the superconducting state.

DC Electrical Resistance

The general behavior of a normal conductor and a superconductor is shown in Figure(1.1) .



Figure(1.1) The general behavior of a normal conductor and a superconductor (Lynn et al., 1988).

The superconducting state is associated with the precipitous drop of the resistance to an immeasurably small value at specific critical temperature T_c . The most familiar property of superconductor is the lack of any resistance to the flow of electrical current. Classically we call this phenomenon perfect conductivity. However, the resistanceless state is much more than just perfect conductivity, and in fact cannot be understood at all on the basis of classical physics, hence the name superconductor.

Now consider initiating a current in a closed loop of wire. For a perfect conductor we might at first expect the current to continue forever. However, the electrons circulating in the loop of wire are in an accelerating reference frame, and an accelerating charge radiates energy. By considering these classical radiation effects a current will decay with time, and hence there is resistance. In a superconductor, their is no observable decay of the supercurrent (with an experimental half-life exceeding 10^5 years)(File and Mills, 1963).

The Meissner Effect

In 1933, it was found that when a superconductor was cooled below T_c in a magnetic field, the magnetic flux was expelled from the superconductor. Thus, in a weak magnetic field, a superconductor has perfect diamagnetism, a phenomenon called the Meissner effect.

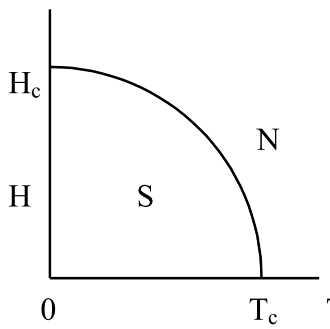
$T > T_c$ $\qquad\qquad$ $T \leq T_c$

Figure(1.2) The Meissner effect (Kittel, 1991).

The Meissner effect implies that in a magnetic field, superconductors develop surface current, which give rise to magnetic fields that exactly cancel the external field, leaving a field-free bulk. The Meissner effect also implies a critical field, H_c, above which superconductivity will be destroyed (Burns, 1992). Experimental values of H_c vs. T are shown in Figure(1.3) The experimental result can be approximately described by a quadratic temperature dependence as

$$H_c(T) = H_c(0)[1-(\frac{T}{T_c})^2] \qquad (1.1)$$

with $H_c(0)$ is a critical magnetic field at 0 K. For a conventional superconductor, $H_c(0)$ values less than 10^3 Oe .



Figure(1.3) Phase diagram in H-T plane, showing superconducting (S) and normal (N) regions, and the critical curve $H_c(T)$ or $T_c(H)$ between them(Lynn et al., 1988).

Magnetic Levitation

One of the most fascinating demonstration of superconductivity is the levitation of a superconducting particle over a magnet (or vice versa). Typically this is done by dropping a particle of superconducting materials in a dish of liquid nitrogen, with a magnet underneath, and watching the particle jumps and hovers above the magnet when the temperature drops below T_c .

The repulsion of the particle from the magnet is caused by the flux exclusion from the interior of the material. We assume for simplicity that the particle is spherical with radius R and that $R >> \lambda_L$, where λ_L is the London penetration depth, so that we may neglect surface effects. We have (Lynn et al., 1988).

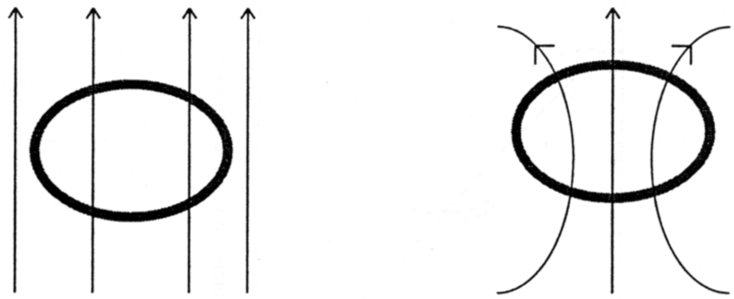
$$h = [\frac{B^2(a)\, a^2}{4\pi\rho g}]^{1/3} \qquad (1.2)$$

where B(a) is the value of the field at the surface of the magnet, a is position of the surface of the magnet, ρ is the density of sphere and h is the height of the sphere above the magnet. We also assume that the average value of B may be taken at center of the sphere ($h >> R$).

Note that this result does not depend on the size of the particle and in fact the only material-dependent parameter is the density . This equation is valid only in the regime that $h >> R >> \lambda_L$.

Flux Quantization

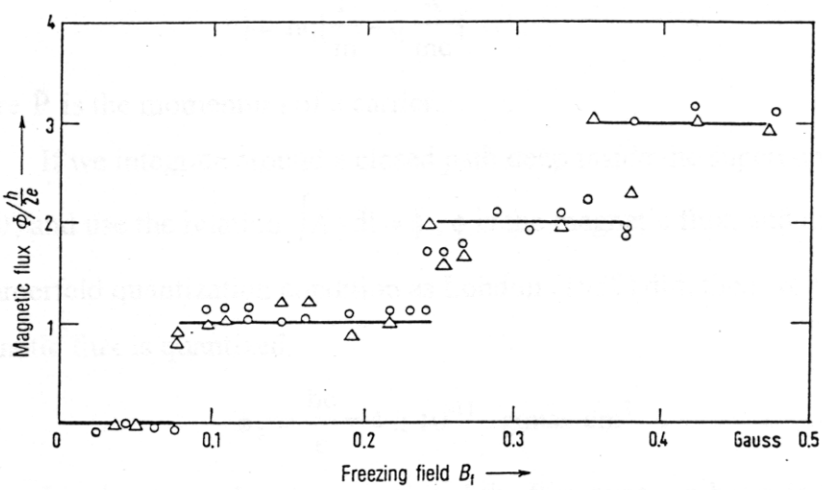
Consider a normal metallic ring placed in magnetic field perpendicular to its plane. When the temperature is lowered, the metal becomes superconducting and expels the flux. Suppose the external field is then removed; no flux can pass through the superconducting metal, and the total trapped flux must remain constant, being maintained by circulating supercurrents in the ring itself. Such persistent currents have been observed over long periods.



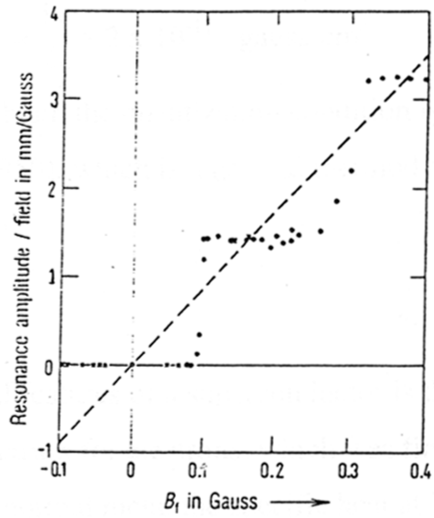
Normal ring in magnetic field Cooled below T_c; magnetic field then remove

Figure(1.4) Flux trapping in a superconducting ring (Kittel, 1991).

Measurements of flux quantization were published by two groups in 1961-Doll and Nabauer (1961) and Deaver and Fairbank(1961) which revealed that the magnetic flux through a superconducting ring can only take up discrete value $n\phi_0$ (n=1,2,3,...). To do this, persistent currents had to be set up in superconducting ring by means of various magnetic fields and the magnetic flux created by these currents were measured so accurately that the resolution revealed the individual quantum jumps. Their results are shown in Figure(1.5).



Figure(1.5a) Results of Deaver and Fairbank (1961) on flux quantization in a cylinder.



Figure(1.5b) Results of Doll and Nabauer (1961) on flux quantization in a Pb cylinder.

London (1950) has already predicted the quantization of the magnetic flux in a superconducting ring for theoretical reasons as 1950. He assumed that a superconducting ring with its persistent current can only take up discrete states which are determined by some sort of quantum conditions.

The current density in any conductor is defined by $\vec{j} = nq\vec{v}$, where n is the density of carriers, q is the charge, $\vec{v}$ is their average velocity and m is the mass . In the presence of a magnetic field we can write this in term of the vector potential $\vec{A}$ as

$$\vec{j} = nq[\frac{\vec{P}}{m} - q\frac{\vec{A}}{mc}] \qquad (1.3)$$

where $\vec{P}$ is the momentum of a carrier.

If we integrate around a closed path deep inside the superconductor where $\vec{j} = 0$, and use the relation $\int \vec{A} \cdot \vec{dl} = \phi$, ϕ is the magnetic flux, and apply the Bohr-Sommerfeld quantization condition as London (1950) did, then we find that the magnetic flux is quantized

$$\phi_0 = \frac{hc}{e} = 4 \text{ x } 10^{-11} \text{ gauss-cm}^2$$

London arrived at this quantity of the flux quantum because he assumed that single electrons carried the supercurrent. Now we know from BCS theory that the supercurrent carried two electrons, Cooper pairs. The flux quantum must be

$$\phi_0 = \frac{hc}{2e} = 2 \text{ x } 10^{-11} \text{ gauss-cm}^2 \qquad (1.4)$$

Another way to obtain the quantization condition is to employ the theory of Ginzburg and Landau (1950), which is a general thermodynamical approach to the theory of phase transition.

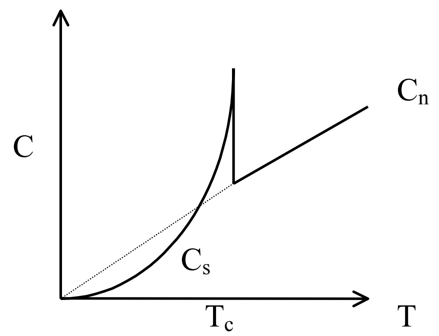
Energy Gap

One of the central features of a superconductor is that there exists an energy gap in the excitation spectrum for electrons, which was first discovered in specific heat measurements. In a normal metal the specific heat at low temperatures is given by (Lynn et al., 1988)

$$C = \gamma T + \beta T^3 \qquad (1.5)$$

where the linear term is due to electron excitations, and cubic term originates from phonon excitation. Below the superconducting transition, the electronic term was found to be of the form $\exp(-\Delta/k_B T_c)$ which is characteristic of a system with a gap in the excitation spectrum of energy 2Δ . The gap is directly related to the superconducting order parameter, and hence we might expect that $\Delta \rightarrow 0$ as $T \rightarrow T_c$.

The transition in zero magnetic field from superconducting state to the normal state is observed to be a second-order phase transition. At a second-order transition there is no latent heat, but there is a discontinuity in the specific heat , evident in Figure(1.6) .



Figure(1.6) Schematic diagram of specific heat in a superconductor.

Isotope Effect

It has been observed that the critical temperature of superconductors varies with isotopic mass smoothly. The experimental results within each series of isotopes may be fitted by a relation of the form (Kittel, 1991)

$$M^{\alpha}T_c = \text{constant} \qquad (1.6)$$

where α is the isotope exponent.

element	Hg	Sn	Cd	Tl	Mo	Os	Ru
Isotope exponent α	0.50	0.47	0.48	0.5	0.33	0.2	0.0

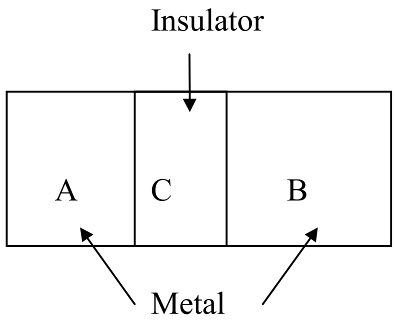
Table(1.2) Isotope exponent of superconductors (Park, 1969).

From the dependence of T_c on the isotope mass we learn that lattice vibrations and electron-lattice interactions are deeply involved in superconductivity. This was a fundamental discovery : there is no other reason for the superconducting transition temperature to depend on the number of neutrons in the nucleus.

The isotope exponent may be lower than 0.5 in superconductor because of the Coulomb repulsion and anharmonicity of phonons. Therefore any finite value of a measured experimentally shows that phonons are involved in the pairing mechanism. However the absence or small isotope effect does not mean that the electron-phonon interaction is irrelevant for superconductivity.

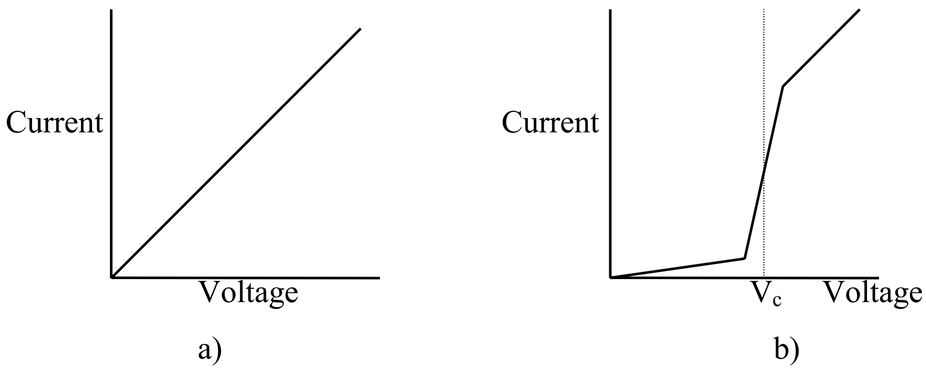
Josephson Superconductor Tunneling

Consider two metals separated by an insulator, as in Figure(1.7). The insulator normally acts as a barrier to the flow of conduction electrons from one metal to the other. If the barrier is sufficient thin (less than 10 or 20 Å) there is a significant probability that an electron which impinges on the barrier will pass from one metal to the other : this is called tunneling.



Figure(1.7) Two metals, A and B, separated by a thin layer of an insulator C (Kittel,1991).

When both metals are normal conductors, the current-voltage relation of the sandwich or tunneling junction is ohmic at low voltages, with the current directly proportional to the applied voltage. Giaever (1960) discovered that if one of the metals becomes superconducting the current-voltage characteristic changes from the straight line of Figure(1.8a) to the curve shown in Figure(1.8b) .



Figure(1.8) a) Linear current-voltage relation for junction of normal metals separated by oxide layer ; b) current-voltage relation with one metal and the other metal superconducting (Kittel,1991).

Under suitable conditions we observe remarkable effects associated with the tunneling of superconducting electron pairs from a superconductor through a layer of an insulator into another superconductor. Such a junction is called a weak link. The effects of pair tunneling include : DC Josephson effect and AC Josephson effect (Kittel,1991).

DC Josephson Effect

When a dc current flows across the junction in the absence of any electric or magnetic field. DC Josephson Effect occurs when wave function of the phase correlation of all Cooper pairs are stricted. In a given superconductor the wave function of the pairs are represented by $\Psi = \Psi_0 \exp(i\theta)$, where θ is the phase and is the same for every pair.Josephson found that the current J of superconducting pairs across the junction depends on the phase difference δ as (Kittel,1991)

$$J = J_0 \sin\delta = J_0 \sin(\theta_2 - \theta_1) \quad (1.7)$$

where J_0 is proportional to the transfer interaction . The current J_0 is the maximum zero-voltage current that can be passed by the junction.

AC Josephson Effect

A dc voltage applied across the junction creates rf current oscillations across the junction. Further, an rf voltage applied with the dc voltage can then cause a dc current across the junction. The current oscillates with frequency

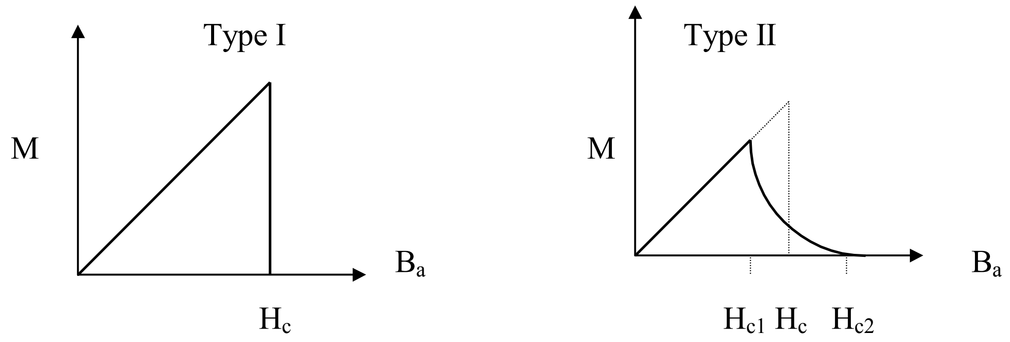
$$\omega = \frac{2eV}{\eta} \quad (1.8)$$

where V is a dc voltage that is applied across the junction and e is the charge of electron..

A dc voltage of 1 μV produces a frequency of 483.6 MHz.

Type of Superconductor

The magnetization curve expected for a superconductor under the conditions of the Meissner-Ochsenfeld experiment is shown in Figure(1.9a) . Above H_c, the specimen is in the normal state and below H_c, it is in the superconducting state. Pure specimens of many materials exhibit this behavior ; they are called type I superconductor or, formerly, soft superconductors. The values of H_c are always too low for type I superconductors to have any useful technical applications.



(a) (b)

Figure(1.9) Magnetization(M) versus applied magnetic field (B_a) for a bulk superconductor a) type I superconductor b) type II superconductor.

Other materials exhibit a magnetization curve of the form of Figure(1.9b) and are known as type II superconductors. They have superconducting electrical properties up to a field denoted by H_{c2} . Above H_{c2}, they are in normal states or are normal conductors. Between the lower critical field H_{c1} and upper critical field H_{c2} the flux density B_0 and the Meissner effect occurs incompletely. In this region, the superconductor is threaded by flux lines and are in the vortex state. The value of H_{c2} may be a hundred times or more higher than the value of critical field H_c of type I superconductor.

Theoretical Survey

There are many theories or models that try to describe the properties of a non-conventional superconductor but they can describe only one or two properties of superconductor. For most of these, there are still useful assumptions and models that are valuable for consideration . It should be the first step of study to reach the theory that can describe high-T_c superconductor (Burns,1992) .

Two-Fluid Model

The superfluid properties of helium (^4He, which has zero electron and nuclear spin and thus is a boson) can be well understood by the two-fluid model. The helium atoms can be considered to be in two states. A fraction of the atoms are in the condensed Bose-Einstein ground state, while the rest are in the normal state. The fraction in the condensed state are assumed to lead to the remarkable properties of superfluid He .

Gorter and Casimer (1934) used this idea of superfluid helium and applied it to superconductivity. The conduction electron density is n = N/V , where N is the number of conduction electrons in the sample of volume V. Then n_n and n_s are the densities of normal-state and superconducting electrons, where $n=n_n+n_s$. Of course, the separation of the conduction electrons in this manner is a drastic assumption. Take $x=n_n/n_s$ and 1-x to be the fractions of normal-state and superconducting-state electrons, respectively. They assumed a free energy for the conduction electrons of the form

$$F(x,T) = x^{1/2} f_n(T) + (1-x) f_s(T) \qquad (1.9)$$

The f_n and f_s terms were taken as

$$f_n(T) = -\frac{\gamma T^2}{2} \qquad (1.10)$$

$$f_s(T) = -\beta \qquad \text{(a constant)} \qquad (1.11)$$

The $\gamma T^2 / 2$ term is the usual free-electron energy in a normal metal that yields a γT (linear) specific heat at low temperatures. The superconducting condensation energy is taken as $-\beta$. At T=0, the free energy is $-\beta$, since all the electrons are in the condensed state, and at $T= T_c$, it is $\gamma T^2 / 2$, since x=1 .

This model can describe the ratio of the electronic specific heat in the superconducting and normal phase well, in agreement with experiment. But the agreements with experiment are not too surprising, since the unusual form for the free energy (Eq.(1.9)) was chosen to yield these results. Nevertheless, two-fluid model gives a physical basis for understanding superconductivity, a useful free energy expression that yields quantities in agreement with experiment.

The London Equation

The brothers F. and H. London (1935) used ideas based on the two-fluid model to try to understand the Meissner effect. Let n, n_n, n_s be the densities of all the conduction electrons, the normal state electrons, and the superconducting electrons, with $n=n_n+n_s$. Assume $n_s(T_c) = 0$ and $n_s(0) = n$. Then, the current due to the superconducting electrons is given by $J = -ev_sn_s$ and from Newton's law, $m\,(dv/dt)= -eE$,

$$\frac{\partial \vec{J}}{\partial t} = \left(\frac{e^2 n_s}{m}\right)\vec{E} \qquad (1.12)$$

$$\vec{E} = \frac{\partial}{\partial t}(\Lambda \vec{J}) \qquad (1.13)$$

where

$$\Lambda = \frac{m}{n_s e^2} \qquad (1.14)\ .$$

Combining these results with Maxwell's equation, $\nabla x \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}$,yields

$$\frac{\partial}{\partial t}[c\nabla x(\Lambda \vec{J}) + \vec{B}] = 0 \qquad (1.15)$$

This general equation for any metal with conduction electron density n_s, will not account for the Meissner effect. The Londons realized that the characteristic behavior of a superconductor could be obtained by restricting the full set of solutions of Eq.(1.15) to those where the expression within the square bracket in Eq.(1.15) is zero, not only its time dependence. Thus

$$\vec{B} = -c\nabla x(\Lambda \vec{J}) \qquad (1.16)$$

which is the London equation, and Λ or n_s can be considered a phenomenological parameter. Taking the curl of both sides, using Maxwell's equation, $\nabla x \vec{B} = \frac{4\pi}{c}\vec{J}$, and using the identity, $\nabla x \nabla x \vec{B} = \nabla(\nabla \cdot \vec{B}) - \nabla^2 \vec{B} = -\nabla^2 \vec{B}$, we obtain

$$\nabla^2 \vec{B} = \frac{\vec{B}}{\lambda_L^2} \qquad (1.17)$$

$$\nabla^2 \vec{J} = \frac{\vec{J}}{\lambda_L^2} \qquad (1.18)$$

where λ_L is the London penetration depth, $\lambda_L = (\frac{m}{4\pi n_s})^{1/2} \frac{c}{e}$.

The specific form of the solution to Eq.(1.17) depends on the particular geometry and boundary condition, but is typically of form $B_0 \exp(-x/\lambda_L)$. Hence Eqs.(1.17) and (1.18) indicate that at an air-superconductor interface, the magnetic field decays from the surface into a superconductor bulk exponentially with a characteristic length scale λ_L . Thus, the London equation gives a simple picture of the Meissner effect ; a current is set up that shields the interior of the sample from the external magnetic field.

Ginzburg-Landau Theory

Ginzburg and Landau (1950) proposed a phenomenological theory of superconductivity, which is related to Landau's theory of second-order phase transition . The free energy is expanded in terms of an order parameter, which is zero in the high-temperature phase. The Ginzburg-Landau, or GL theory, introduces a complex pseudo-wave function ψ as the order parameter, which is hypothesized to be related to the local density of superconducting electrons as

$$n_s \equiv \frac{N_s}{V} = |\psi(r)|^2 \qquad (1.19)$$

and n_s is the conduction band electron density.

Near the critical temperature $\Psi(r)$ is small and the Gibbs free energy (Ω) may be expand into a series in $\Psi(r)$. In the absence of magnetic fields and in the absence of spatial variations, the free energy density between the superconducting and normal state is taken as

$$\Omega_s = \Omega_n + a|\Psi|^2 + \frac{1}{2} b|\Psi|^4 + \ldots \qquad (1.20)$$

Since the theory is built up for the vicinity of T_c, the coefficients a and b can be expand in $\tau=(T-T_c)/T_c$ and only the first nonvanishing terms need be retained. Since the minimum of Ω_s corresponds to $\Psi=0$ above T_c and $\Psi \neq 0$ below T_c , the coefficient a change sign at the transition point; therefore, $a = \alpha\tau$, where $\alpha > 0$. From the condition that $\Psi=0$ must correspond to the minimum of Ω_s at the transition point too, we have $b \approx b(T_c) > 0$ .Differentiating with respect to Ψ^*, we obtain the condition of the minimum of Ω_s ;

$$\Psi(\alpha\tau + b|\Psi|^2) = 0 \tag{1.21}$$

This yields the equilibrium value :

$$\Psi = 0 \quad , \qquad T > T_c$$

$$|\Psi(r)|^2 = -\alpha\tau / b \, , \qquad T < T_c$$

Substituting the equilibrium value into Eq.(1.20),

$$\Omega_s - \Omega_n = -\frac{(\alpha\tau)^2}{b} + \frac{1}{2}\frac{(\alpha\tau)^2}{b} = -\frac{(\alpha\tau)^2}{2b} \tag{1.22}$$

Since we consider the equilibrium in a given field, we have to use the formula for F_H where $F_H = F_0 - \frac{\mu H^2}{8\pi}$, F_0 is free energy without magnetic field and F_H is the free energy in the magnetic field.The magnetic field can penetrates a normal metal completely and superconducting metals are nonmagnetic, therefore $\mu=1$. Hence, $F_n(H_c, T) = F_n - \frac{H_c^2}{8\pi}$. From this we see that magnetic contribution to F_n is much larger than that to F_s. We have the condition for the superconducting transition that is $F_s(H_c, T) = F_n(H_c, T)$. We obtain

$$F_n(T) - F_s(T) = \frac{H_c^2}{8\pi} \tag{1.23}$$

Comparing Eq.(1.23) with Eq.(1.22), we have

$$\Omega_n - \Omega_s = \frac{(\alpha\tau)^2}{2b} = \frac{H_{cm}^2}{8\pi} \tag{1.24}$$

where H_{cm} is the thermodynamic critical field of a bulk superconductor. From this equation, we can also derive a microscopic formula for a certain combination of coefficient α and b .

Suppose now that an external magnetic field is applied to the superconductor. In this case, both the field in superconductor and Ψ depend on the coordinates. We will assume that the variation of Ψ in space occurs slowly then

$$|\Psi|^2 = (\Psi_0^* + \nabla\Psi_0^* + \ldots)(\Psi_0 + \nabla\Psi_0 + \ldots) \approx |\Psi|^2 + |\nabla\Psi|^2$$

Here, we permit one to consider only the correction $|\nabla\Psi|^2$ to the free energy and

$\Psi_0 \approx \Psi$. The momentum operator $-i\eta\nabla$ must necessarily be included in the combination $(-i\eta\nabla - (\frac{2e}{c})\vec{A})$, where A is the vector potential and we take into account that the pair has a charge $2e$ .So we can get the kinetic energy of a particle of mass $2m$ as $\frac{1}{4m}\left|(-i\eta\nabla - \frac{2e}{c}A)\Psi\right|^2$.

The free energy in the present of magnetic field can be written as

$$\Omega_s = \Omega_n + \alpha\tau|\Psi|^2 + \frac{1}{2}b|\Psi|^4 + \frac{1}{4m}\left|(-i\eta\nabla - \frac{2e}{c}\vec{A})\Psi\right|^2 + \frac{H^2}{8\pi} \qquad (1.25)$$

The total free energy , Ω_t , equal to $\Omega_t = \int \Omega_s dv$.

In order to obtain the minimum of the total free energy, we vary Ω_t with respect to Ψ^* and we obtain

$$\int \left\{ \delta\Psi^*\alpha\tau\Psi + \delta\Psi^* b|\Psi|^2\Psi + \frac{\delta\Psi^*}{4m}(i\eta\nabla - \frac{2e}{c}\vec{A})(-i\eta\nabla - \frac{2e}{c}\vec{A})\Psi \right\} dv = 0$$

or

$$\int \delta\Psi^* \left\{ \alpha\tau\Psi + b|\Psi|^2\Psi + \frac{1}{4m}\left|-i\eta\nabla - \frac{2e}{c}\vec{A}\right|^2 \Psi \right\} dv = 0 \qquad (1.26)$$

The variation of $\delta\Psi^*$ is arbitrary, For $\delta\Psi^* = 0$ at the surface, we get

$$\int \delta\Psi^* (\alpha\tau\Psi + b|\Psi|^2\Psi + \frac{1}{4m}(-\frac{2e}{c})\vec{A}(-i\eta\nabla - \frac{2e}{c}\vec{A})\Psi) dv = 0 \qquad (1.27)$$

For $\delta\Psi^*$ is arbitrary at surface, we get

$$\frac{\delta\Psi^*}{4m}\int i\eta\nabla \cdot (-i\eta\nabla - \frac{2e}{c}\vec{A})\Psi dv = 0 \qquad (1.28)$$

We find that

$$\frac{1}{4m}(-i\eta\nabla - \frac{2e}{c}\vec{A})^2\Psi + \alpha\tau\Psi + b|\Psi|^2\Psi = 0 \qquad (1.29)$$

Applying Guauss's law, $\oint \hat{n} \cdot \vec{A} ds = \int \nabla \cdot \vec{A} dv$, to Eq.(1-28), we get

$$\hat{n} \cdot (-i\eta\nabla - \frac{2e}{c}\vec{A})\Psi\Big|_{surface} = 0 \qquad (1.30)$$

Eq.(1.30) is the boundary condition of Eq.(1.29). The meaning of these equations is that the current perpendicular to surface equal to zero.

Now we vary Ω_t with respect to the vector potential A, assuming that $\vec{H} = \nabla x \vec{A}$. The variation of H^2 gives $2\nabla x(\vec{A}\nabla x\delta\vec{A})$. We may use the formula $\nabla\cdot(\vec{a}\vec{b}) = \vec{b}\cdot\nabla x\vec{a} - \vec{a}\cdot\nabla x\vec{b}$. This yields $2\delta\vec{A}\nabla x\nabla x\vec{A} + 2\nabla\cdot(\delta\vec{A}\nabla x\vec{A})$. The volume integral of div is transformed to a surface integral and vanishes.Equating the variation to zero, we find

$$\nabla x\nabla x\vec{A} = \nabla x\vec{H} = \frac{4\pi}{c}\vec{j} \tag{1.31}$$

and

$$\vec{j} = -\frac{ie\eta}{2m}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) - \frac{2e^2}{mc}|\Psi|^2\vec{A} \tag{1.32}$$

Eq.(1.31) is a Maxwell's equation. The boundary condition is the specification of the field at the superconductor surface. Expression (1.32) corresponds to the quantum-mechanical current in the magnetic field if the wave function is equal to Ψ, the charge is 2e and the mass 2m .

We now pass over to new units which will allow us to drop most of the constants in Eqs.(1.29)-(1.32). We introduce the following notation :

$$\Psi' = \frac{\Psi}{\Psi_0} \qquad H' = \frac{H}{\sqrt{2}H_{cm}}$$

$$r' = \frac{r}{\delta} \qquad \delta = \sqrt{\frac{2mc^2}{4\pi\Psi_0^2(2e)^2}} \qquad \Psi_0^2 = \frac{\alpha|\tau|}{b} \tag{1.33}$$

$$A' = \frac{A}{\sqrt{2}\delta H_{cm}} \qquad H_{cm} = \frac{2\alpha\tau\sqrt{\pi}}{\sqrt{b}}$$

As a result, the equations become

$$\left(\frac{-i\nabla}{\chi} - \vec{A}\right)^2\Psi - \Psi + |\Psi|^2\Psi = 0 \tag{1.34}$$

$$\vec{n}\cdot\left(\frac{-i\nabla}{\chi} - \vec{A}\right)\Psi\Big|_{surface} = 0 \tag{1.35}$$

and
$$\nabla x\nabla x\vec{A} = \frac{-i}{2\chi}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) - |\Psi|^2\vec{A} \tag{1.36}$$

Equations (1.34), (1.35), and (1.36) contain only one constant, χ, which is called the Ginzburg-Landau parameter ; it is defined as $\chi = 2^{3/2}eH_{cm}\delta^2/\eta c$.

In the vicinity of T_c, we have

$\chi < \frac{1}{\sqrt{2}}$ for type I superconductor

$\chi > \frac{1}{\sqrt{2}}$ for type II superconductor

Let us consider the simplest case : the penetration of a weak magnetic into the bulk of a superconductor with a planar boundary. Let the superconductor occupy the half-space x=0 . The field is applied to it along the z axis. The field penetrates the superconductor and decreases rapidly in the bulk, it depends on x . Therefore, we choose the vector potential $\vec{A}$ along the direction y.

$$\vec{H} = \nabla x \vec{A} = \frac{dA_y}{dx}\vec{k} \qquad (1.37)$$

It is natural to assume that is also depend only on x . We obtain the Ginzburg-Landau as

$$-\chi^2 \frac{d^2\psi}{dx^2} - \psi + A^2\psi + |\psi|^2 \psi = 0 \qquad (1.38)$$

and
$$\left.\frac{d\psi}{dx}\right|_{surface} = 0 \qquad (1.39)$$

Then we obtain $|\psi|^2 \cong 1 - A^2 \cong 1$ or Ψ= constant. Eq.(1.36) yield

$$\frac{d^2}{dx^2}A - A = 0 \qquad (1.40)$$

We can get $A = A_0\, e^{-x}$.

Differentiating with respect to x, we derive a similar equation for H. the solution that satisfies the boundary condition $H = H_0$ then $H = H_0\, e^{-x}$ or , in conventional unit $H = H_0\, e^{-x/\delta}$ where δ is the London penetration depth near T_c . In this case, we get δ =1 . Substitution δ into Eq.(1.33), we will find the relation of T_c, H_c and the other that can describe the properties of superconductor .

Using the GL theory, we are able to obtain a temperature-dependent coherence length (ξ) besides a temperature-dependent penetration depth (λ) . The importance GL parameter is the ratio of these two lengths,

$$\chi \equiv \frac{\lambda}{\xi} \tag{1.41}$$

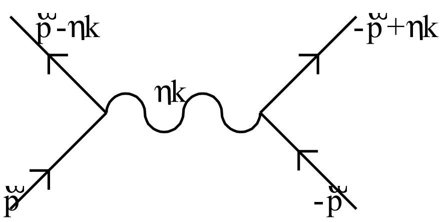
For the most of conventional superconductor, $\chi \ll 1$ and for all high-T_c superconductor, $\chi \gg 1$.

When first proposed, the GL theory was not thought to be particularly important.Because it cannot explain what is the meaning and mechanism of occurring of order parameter. Today, the GL theory is not only appreciated, it is essentially the only way to deal with spatially inhomogeneous systems such as thin films, proximity system, and others.

CHAPTER II

BCS THEORY

We consider the theory introduced by Bardeen, Cooper, and Schrieffer (BCS) in 1957 (Bardeen, Cooper, and Schrieffer, 1957). The BCS theory has been very successful in describing conventional superconductors. It is based on the idea that in the superconducting state, the electrons near the Fermi surface have a mutual attraction. This attraction was due to polarization of the ionic lattice by the electron (the electron-phonon-electron interaction). An attractive force among electrons combines two electrons with momenta $\vec{p}$ and $-\vec{p}$ into a Cooper pair (Cooper, 1956).



Figure(2.1) The electron-phonon interaction

The BCS theory incorporates the assumption of a weak net attractive force. The BCS ground-state wavefunction for the many electrons is an antisymmetrized product of identical, pair wavefunctions, where each pair wavefunction has a total momentum of zero and a total spin of zero. The simple model (Golovashkin et al., 1981) which permits such behavior is given by the BCS "reduced" Hamiltonian, $H = H_0 - H_{red}$, where

$$H_0 = \sum_{k\sigma} \varepsilon_k C^{+}_{k\sigma} C_{k\sigma} \qquad (2.1)$$

$$H_{red} = \sum_{kk'} V_{kk'} C^{+}_{k\uparrow} C^{+}_{-k\downarrow} C_{-k'\downarrow} C_{k'\uparrow} \quad . \tag{2.2}$$

where ε_k is the energy of the conduction electron above Fermi energy. $C^{+}_{k\sigma}(C_{k\sigma})$ is the creation (annihilation) operator for electron. $V_{kk'}$ is interaction matrix element. σ is spin index. Interaction in Eq.(2.2) contain terms that scatter pairs of electron from one pair state $(k\uparrow,-k\downarrow)$ to a different one $(k'\uparrow,-k'\downarrow)$. The interaction matrix elements $V_{kk'}$ are at this state unspecified. Bardeen, Cooper and Schrieffer had in mind the Frohlich or Bardeen-Pines (Bardeen and Pines, 1955) effective phonon-induced interaction which $V_{kk'}$ is negative.

The characteristic BCS pair-interaction Hamiltonian will lead to a ground state which is some phase-coherent superposition of many-body states with pairs of state $(k\uparrow,-k\downarrow)$ occupied or unoccupied as unit. Because of the coherence, operators such as $C_{-k\downarrow}C_{k\uparrow}$ can have nonzero expectation values $< C_{-k\downarrow}C_{k\uparrow} >$. The bracket $< >$ denotes the thermal average. We define

$$\Delta = \sum_{k} V_k < C_{-k\downarrow} C_{k\uparrow} > \tag{2.3}$$

In terms of Δ, the model Hamiltonian becomes

$$H = \sum_{k\sigma} \varepsilon_k C^{+}_{k\sigma} C_{k\sigma} + \sum_{k} \Delta (C^{+}_{k\uparrow} C^{+}_{-k\downarrow} + \text{h.c.}) \tag{2.4}$$

here h.c. is hermitian conjugate .

We define the Green's function as

$$G(k,\omega_n) =< -T\tau \Psi_k(\tau) \Psi^{+}_k(0) >=< -T_\tau \begin{pmatrix} C_{k\uparrow}C^{+}_{k\uparrow} & C_{k\uparrow}C_{-k\downarrow} \\ C^{+}_{-k\downarrow}C^{+}_{k\uparrow} & C^{+}_{-k\downarrow}C_{-k\downarrow} \end{pmatrix} >$$

$$= \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix} \tag{2.5}$$

where $\Psi_k^+ = (C_{k\uparrow}^+ \quad C_{-k\downarrow})$ and T_τ is the time ordering operator for the imaginary time τ =it .

Using the Heisenberg's equation of motion for the creation and annihilation operators with the BCS Hamiltonian.We get

$$i\frac{d}{dt}C_{k\uparrow} = [C_{k\uparrow}, H] \ .$$

$$= \varepsilon_k C_{k\uparrow} - \Delta C_{-k\downarrow}^+$$

then

$$(i\frac{d}{dt} - \varepsilon_k)C_{k\uparrow} + \Delta C_{-k\downarrow}^+ = 0 \qquad (2.5.1)$$

Proceeding in the same manner for $C_{-k\downarrow}^+$,we obtain the equation :

$$(i\frac{d}{dt} + \varepsilon_k)C_{-k\downarrow}^+ + \Delta C_{k\uparrow} = 0 \qquad (2.5.2)$$

By Fourier transforming Eq.(2.5.1), we obtain the matrix elements of the Green's function as

$$(i\omega_n - \varepsilon_k) < -T_\tau C_{k\uparrow} C_{k\uparrow}^+ > +\Delta < -T_\tau C_{-k\downarrow}^+ C_{k\uparrow}^+ >= [C_{k\uparrow}, C_{k\uparrow}^+]$$

or

$$(i\omega_n - \varepsilon_k)G_{11} + \Delta G_{21} = 1 \qquad (2.5.3)$$

Similarly from Eq.(2.5.2), we can get

$$(i\omega_n + \varepsilon_k)G_{21} + \Delta G_{11} = 0 \qquad (2.5.4)$$

where ω_n=(2n+1)πT with n is integer and T as temperature. Eqs.(2.5.3) and (2.5.4) can be written in matrix form as

$$\begin{bmatrix} i\omega_n - \varepsilon_k & \Delta \\ \Delta & i\omega_n + \varepsilon_k \end{bmatrix} \begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix} = 1 \qquad (2.5.5)$$

We find the single particle Green's function of a superconductor as

$$G(k,\omega_n) = (i\omega_n - \varepsilon_k\tau_3 + \Delta\tau_1)^{-1} \qquad (2.6)$$

where τ_1 and τ_3 are Pauli matrices with $\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

Because of the relation $\Delta = \sum_k V_k < C_{-k\downarrow}C_{k\uparrow} >$, we can rewrite Δ to be a function of the Green's function as

$$\Delta = \sum_k V_k G_{21}(k,\omega_n) \qquad (2.7)$$

Using the Green's function of a superconductor and for constant interaction potential V_k=V and constant density of state N(ε)=N(0), we get

$$\Delta = 2T\sum_{k=0}^{\infty}\sum_n V\frac{\Delta}{\omega_n^2 + \varepsilon_k^2 + \Delta^2}$$

$$= 2N(0)TV\int_0^{\omega_D} d\varepsilon\, \Delta\sum_n \frac{1}{\omega_n^2 + \varepsilon_k^2 + \Delta^2} \qquad (2.8)$$

Using $\sum_n \frac{T}{\omega_n^2 + E_k^2} = \sum_n \frac{T}{2E_k}\left(\frac{1}{i\omega_n + E_k} - \frac{1}{i\omega_n - E_k}\right)$

where $E_k = \sqrt{\varepsilon_k^2 + \Delta^2}$ is the energy of one-particle of Cooper pair.

We calculate the frequency sum of form $\sum_n \frac{1}{i\omega_n + E_k}$. We require a meromorphic function with the same poles as

$$T\sum_n f(i\omega_n) = -\oint \frac{dz}{2\pi i} n_F(z) f(z)$$

where $n_F(z) = \frac{1}{e^{z/T}+1}$ is fermion distribution function.

The integration can be performed by using the residue theorem and we get

$$\sum_n \frac{T}{\omega_n^2 + E_k^2} = \frac{1}{2E_k}\tanh(\frac{E_k}{2T})$$

Substitution this equation in Eq.(2.8) ,

$$\Delta = \lambda \int_0^{\omega_D} \Delta \frac{\tanh(\frac{\sqrt{E_k^2+\Delta^2}}{2T})}{\sqrt{E_k^2+\Delta^2}} dE_k$$

where λ=N(0)V .

If Δ does not depend on electron energy , we write

$$\frac{1}{\lambda} = \int_0^{\omega_D} \frac{\tanh(\frac{\sqrt{E_k^2+\Delta^2}}{2T})}{\sqrt{E_k^2+\Delta^2}} dE_k \quad . \qquad (2.9)$$

BCS Gap and Critical Temperature

It follows from the above consideration that the BCS superconductivity is linked with the order parameter Δ , which is defined as a gap in the quasiparticle spectrum.

At T=0 ,order parameter Δ(T) = Δ(0) and tanh(1/T) =1, the nontrivial solution of Eq.(2.9) is determined from

$$\frac{1}{\lambda} = \int_0^{\omega_D} \frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta^2(0)}} = \sinh^{-1}(\frac{\omega_D}{\Delta(0)}) \qquad (2.10)$$

applying the approximation $\sinh^{-1}(\frac{x}{2}) \cong \ln(x)$, when x>>1 which is applicable in this case because we consider the weak-coupling limit, ω_D >> Δ , then

$$\frac{1}{\lambda} = \ln(\frac{2\omega_D}{\Delta(0)}) \quad \text{or} \quad \Delta(0) = 2\omega_D e^{-1/\lambda} \qquad (2.11)$$

for $\lambda<<1$, the limit to which the theory is applied.

At $T = T_c$, $\Delta(T_c) = 0$. T_c is determined by the equation,

$$\frac{1}{\lambda} = \int_0^{\omega_D} \frac{\tanh(\varepsilon / 2T_c)}{\varepsilon} d\varepsilon$$

$$= (\ln\varepsilon \tanh(\varepsilon)) \Big|_0^{\omega_D/2T_c} - \int_0^{\omega_D/2T_c} \ln\varepsilon \operatorname{sech}^2\varepsilon d\varepsilon \qquad (2.12)$$

Because $\omega_D >> T_c$ then we replace $\int_0^{\omega_D/2T_c}$ by $\int_0^{\infty}$ and $\tanh(\omega_D/2T_c) \cong 1$ .We get $\int_0^{\infty} \ln\varepsilon \operatorname{sech}^2\varepsilon d\varepsilon = \ln(\frac{\pi}{4\gamma})$ where $\gamma = e^C = 1.78$ and $C \cong 0.577$ is the Euler's constant. Eq.(2.12) because

$$\frac{1}{\lambda} = \ln(\frac{\omega_D}{2T_c}) - \ln(\frac{\pi}{4\gamma})$$

$$= \ln(\frac{2\gamma}{\pi}\frac{\omega_D}{T_c}) \qquad (2.13)$$

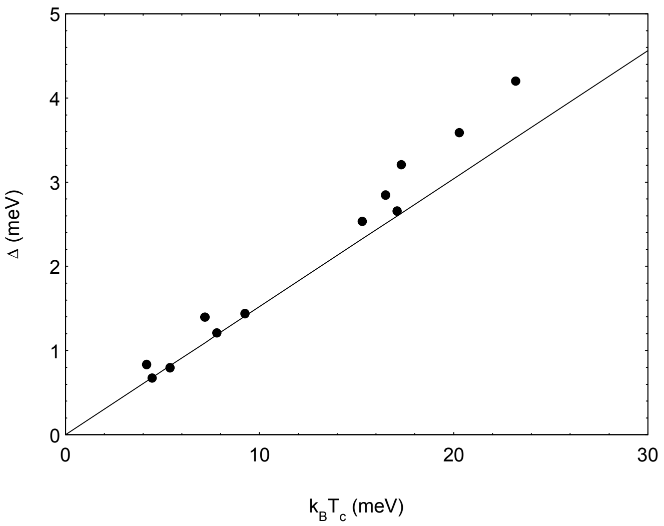
or

$$T_c = (\frac{2\gamma}{\pi})\omega_D e^{-1/\lambda} = 1.14\omega_D e^{-1/\lambda} \qquad (2.14)$$

Therefore Eq. (2.14) and Eq. (2.11) give the gap-to-T_c ratio as

$$\frac{2\Delta(0)}{T_c} = \frac{2\pi}{\gamma} = 3.52 \qquad (2.15)$$

This is the BCS 's universal ratio of a superconductor.



Figure(2.2) Comparing measured energy gap of superconductor (dot) to the calculated gap of BCS theory (solid line).

From Figure(2.2), we find that the BCS predicted that superconductors with large Δ(0) have large T_c . But this prediction does not agree well with the experimental data of superconductor with T_c in higher region (about 30 K).

At very low temperature $T \ll T_c$ $(T \neq 0)$ and let $\Delta(T) = \Delta(0) + \Delta_1(T)$ where $\Delta_1(T) \ll \Delta(0)$, we expand

$$\tanh\left(\frac{\sqrt{\varepsilon^2+\Delta^2(T)}}{2T}\right) \cong \tanh\left(\frac{\sqrt{\varepsilon^2+\Delta^2(0)}}{2T}\right)$$

$$\cong 1 - 2e^{\frac{-\sqrt{\varepsilon^2+\Delta^2(0)}}{T}}$$

$$\cong 1 - 2e^{-\left(\frac{\Delta(0)}{T}+\frac{\varepsilon^2}{2T\Delta(0)}\right)}$$

Substitution of these equations into Eq.(2.9) yields

$$\frac{1}{\lambda} \cong \int_0^{\omega_D} \frac{1}{\sqrt{\varepsilon^2+\Delta^2(T)}} d\varepsilon - e^{-\Delta(0)/T} \int_0^{\omega_D} \frac{e^{-\varepsilon^2/2T\Delta(0)}}{\sqrt{\varepsilon^2+\Delta^2(0)}} d\varepsilon$$

$$\cong \ln\left(\frac{2\omega_D}{\Delta(T)}\right) - 2e^{-\Delta(0)/T} \int_0^{\omega_D/\sqrt{2T\Delta(0)}} \frac{e^{-x^2}}{\sqrt{x^2+\Delta(0)/2T}} dx$$

We take $\omega_D/T_c \to \infty$ and $\frac{\Delta(0)}{2T} >> \frac{\omega_D}{\sqrt{2T\Delta(0)}}$,we can get

$$\int_0^{\omega_D/\sqrt{2T\Delta(0)}} \frac{e^{-x^2}}{\sqrt{x^2+\Delta(0)/2T}} dx \cong \sqrt{\frac{2T}{\Delta(0)}} \int_0^{\infty} e^{-x^2} dx = \sqrt{\frac{\pi T}{2\Delta(0)}}$$

since $\frac{1}{\lambda} = \ln(\frac{2\omega_D}{\Delta(0)})$, we find that

$$\ln(\frac{2\omega_D}{\Delta(0)}) - \ln(\frac{2\omega_D}{\Delta(T)}) = -\sqrt{\frac{2\pi T}{\Delta(0)}} \quad e^{-\Delta(0)/T}$$

By using the approximation

$$\ln(\frac{\Delta(T)}{\Delta(0)}) = \ln(1+\frac{\Delta_1(T)}{\Delta(0)}) \cong \frac{\Delta_1(T)}{\Delta(0)}$$

We then find the relation between $\Delta(0)$ and $\Delta_1(T)$ as

$$\Delta_1(T) = -\sqrt{2\pi T\Delta(0)} \quad e^{-\Delta(0)/T}$$

and

$$\Delta(T) = \Delta(0) - \sqrt{2\pi T\Delta(0)} \quad e^{-\Delta(0)/T} \qquad (2.16)$$

In the vicinity of T_c where $(T_c\text{-}T)/T_c << 1$ the gap is small compared with temperature. However direct expansion in powers of Δ cannot be applied to Eq. (2.9) . Instead it is convenient to use

$$\frac{\tanh x}{x} = \sum_{n=-\infty}^{\infty} \frac{1}{x^2 + (\pi(n+1/2))^2}$$

Substitution this relation into Eq.(2.9) yields

$$\frac{1}{\lambda} = 4T \sum_{n=0}^{\omega_D/2\pi T} \int_0^{\omega_D} \frac{1}{\varepsilon^2 + \Delta^2 + \omega_n^2} d\varepsilon \qquad (2.17)$$

where $\omega_n=\pi T(2n+1)$, ω_n is Matsubara frequency , n=0,1,2,3,...

We expand $\frac{1}{\varepsilon^2+\Delta^2+\omega_n^2}$ in powers of Δ , and get

$$\frac{1}{\varepsilon^2+\Delta^2+\omega_n^2} \cong \frac{1}{\varepsilon^2+\omega_n^2} - \frac{\Delta^2(T)}{(\varepsilon^2+\omega_n^2)^2} .$$

Substituting the approximation in Eq.(2.17) , we find

$$\frac{1}{\lambda} = 4T\sum_{n=0}^{\omega_D/2\pi T}\left(\int_0^{\omega_D}\frac{1}{\varepsilon^2+\omega_n^2}d\varepsilon - \int_0^{\omega_D}\frac{\Delta^2(T)}{(\varepsilon^2+\omega_n^2)}d\varepsilon\right) \quad (2.18)$$

But we have $\frac{1}{\lambda} = \ln(\frac{2\omega_D\gamma}{\pi T_c})$.

Consider the first term on right-hand side of Eq.(2.18) and take $\int_0^{\omega_D} \to \int_0^{\infty}$, we get

$$4T\sum_{n=0}^{\omega_D/2\pi T}\int_0^{\infty}\frac{1}{\varepsilon^2+\omega_n^2}d\varepsilon = 2T\sum_{n=0}^{\omega_D/2\pi T}\frac{\pi}{\pi T(2n+1)} = \ln(\frac{2\omega_D\gamma}{\pi T})$$

by using the formula $\int_0^{\infty}\frac{1}{x^2+a^2}dx = \frac{\pi}{2a}$.

Consider the second term on right-hand side of Eq.(2.18) and take $\int_0^{\omega_D} \to \int_0^{\infty}$ and $\sum_{n=0}^{\omega_D/2\pi T} \to \sum_{n=0}^{\infty}$, we get

$$-4T\sum_{n=0}^{\infty}\int_0^{\infty}\frac{\Delta^2(T)}{(\varepsilon^2+\omega_n^2)^2}d\varepsilon = \frac{-\Delta^2(T)}{\pi^2T^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^3}$$

$$= -\frac{\Delta^2(T)}{\pi^2T^2}\frac{7}{8}\zeta(3) .$$

By using the relation $\int_0^{\infty}\frac{1}{(x^2+a^2)^2}dx = \frac{\pi}{4a^3}$ and $\zeta(x) = \sum_{n=1}^{\infty}\frac{1}{n^x}$, is the Riemann zeta function

and $$\sum_{n=0}^{\infty}\frac{1}{(2n+1)^3} = 1+\frac{1}{2^3}+\frac{1}{3^3}+\frac{1}{4^3}+\ldots-[\frac{1}{2^3}+\frac{1}{4^3}+\frac{1}{6^3}+\ldots]$$

$$= \zeta(3) - \frac{1}{2^3}(1 + \frac{1}{2^3} + \frac{1}{3^3} + \ldots)$$

$$= \frac{7}{8}\zeta(3) \ .$$

Substitution these equation into Eq.(2.18), we get

$$\ln(\frac{2\omega_D\gamma}{\pi T_c}) = \ln(\frac{2\omega_D\gamma}{\pi T}) - \frac{7}{8}\zeta(3)\frac{\Delta^2(T)}{\pi^2 T^2}$$

or $$\ln(\frac{T}{T_c}) = -\frac{7}{8}\zeta(3)\frac{\Delta^2(T)}{\pi^2 T^2} \ .$$

Because T is near T_c, we can use the relation

$$\ln(\frac{T}{T_c}) = \ln(1 + (\frac{T - T_c}{T_c})) \cong \frac{T - T_c}{T_c} \ .$$

So we get

$$\Delta^2(T) = (\frac{T_c - T}{T_c})\pi^2 T_c^{\ 2}(\frac{8}{7\zeta(3)}) \tag{2.19}$$

or

$$\Delta(T) = \pi(T_c(T_c - T))^{1/2}\sqrt{\frac{8}{7\zeta(3)}} \quad ,\zeta(3) = 1.20206$$

$$= 3.06\sqrt{T_c(T_c - T)} \tag{2.20}$$

Thermodynamic function

In the uniform system, the thermodynamic potential in the normal state and superconducting state are Ω_n ,Ω_s respectively. A relation between Ω_n and Ω_s can be written as

$$\Omega_s - \Omega_n = -v\int_0^{\Delta} d\Delta'(\Delta')^2 \frac{d(1/V)}{d\Delta'} \tag{2.21}$$

where v is volume of material and V is the interaction potential where

$$\frac{1}{V} = N(0) \int_0^{\omega_D} \frac{\tanh(\sqrt{\varepsilon^2 + \Delta^2} / 2T)}{\sqrt{\varepsilon^2 + \Delta^2}} d\varepsilon$$

then

$$\frac{\Omega_s - \Omega_n}{v} = N(0) \int_0^{\omega_D} d\varepsilon \int_0^{\Delta} d\Delta'(\Delta')^2 \frac{d}{d\Delta'} \left(\frac{\tanh(\sqrt{\varepsilon^2 + \Delta'^2} / 2T)}{\sqrt{\varepsilon^2 + \Delta'^2}} \right).$$

$$= N(0) \int_0^{\omega_D} d\varepsilon \left[\frac{\Delta^2}{\sqrt{\varepsilon^2 + \Delta^2}} \tanh(\sqrt{\varepsilon^2 + \Delta^2} / 2T) - 2\int_0^{\Delta} d\Delta' \frac{\Delta'}{\sqrt{\varepsilon^2 + \Delta'^2}} \tanh(\sqrt{\varepsilon^2 + \Delta'^2} / 2T) \right] .$$

Consider the second term on right-hand side and use the method of changing variable $x = \sqrt{\varepsilon^2 + \Delta^2} \Rightarrow$ so that $dx = \frac{\Delta}{x} d\Delta$

$$= 2 \int_{\varepsilon}^{\sqrt{\varepsilon^2 + \Delta^2}} \frac{x}{\Delta'} \cdot \frac{\Delta'}{x} \tanh\left(\frac{x}{2T}\right) dx = 4T \ln\left(\frac{\cosh(\sqrt{\varepsilon^2 + \Delta^2} / 2T)}{\cosh(\varepsilon / 2T)} \right) .$$

We have

$$\ln\left[\frac{\cosh(\sqrt{\varepsilon^2 + \Delta^2} / 2T)}{\cosh(\varepsilon / 2T)} \right] = \ln\left[\frac{e^{\sqrt{\varepsilon^2+\Delta^2}/2T} + e^{-\sqrt{\varepsilon^2+\Delta^2}/2T}}{e^{\varepsilon/2T} + e^{-\varepsilon/2T}} \right]$$

$$= \ln(e^{\sqrt{\varepsilon^2+\Delta^2}/2T - \varepsilon/2T}) + \ln\left(\frac{1 + e^{-\sqrt{\varepsilon^2+\Delta^2}/T}}{1 + e^{-\varepsilon/T}} \right)$$

$$= \frac{1}{2T}(\sqrt{\varepsilon^2 + \Delta^2} - \varepsilon) + \ln(1 + e^{-\sqrt{\varepsilon^2+\Delta^2}/T}) - \ln(1 + e^{-\varepsilon/T})$$

then

$$\frac{\Omega_s - \Omega_n}{v} = \frac{\Delta^2}{V} - 2N(0) \int_0^{\omega_D} (\sqrt{\varepsilon^2 + \Delta^2} - \varepsilon) d\varepsilon - 4N(0)T \int_0^{\omega_D} \ln(1 + e^{-\sqrt{\varepsilon^2+\Delta^2}/T}) d\varepsilon$$

$$+4N(0)T \int_0^{\omega_D} \ln(1 + e^{-\varepsilon/T}) d\varepsilon \qquad (2.22)$$

Because $\omega_D >> T$, we can approximate the integration $\int_0^{\omega_D}$ by $\int_0^{\infty}$, then

$$\int_0^{\infty} \ln(1 + e^{-\varepsilon/T}) d\varepsilon = \frac{1}{12}\pi^2 T$$

and

$$\int_0^{\omega_D} (\sqrt{\varepsilon^2+\Delta^2}-\varepsilon)d\varepsilon = \int_0^{\sinh^{-1}(\omega_D/\Delta)} \Delta^2 \cosh^2\theta d\theta - \frac{\omega_D^2}{2}$$

$$= \frac{\Delta^2}{2}[\sinh^{-1}(\omega_D/\Delta) + \frac{\omega_D}{\Delta}\sqrt{1+(\omega_D/\Delta)^2}] - \frac{\omega_D^2}{2}$$

$$\cong \frac{\Delta^2}{4} + \frac{\Delta^2}{2}\ln(\frac{2\omega_D}{\Delta})$$

$$= \frac{\Delta^2}{4} + \frac{\Delta^2}{2}\ln(\frac{2\omega_D}{\Delta}) + \frac{\Delta^2}{2}(\frac{1}{N(0)V} - \ln(\frac{2\omega_D}{\Delta(0)}))$$

$$= \frac{\Delta^2}{4} + \frac{\Delta^2}{2N(0)V} + \frac{\Delta^2}{2}\ln(\frac{\Delta(0)}{\Delta})$$

Substitution of this integration into Eq.(2.22), we get

$$\frac{\Omega_s - \Omega_n}{v} = -\frac{1}{2}N(0)\Delta^2 - \Delta^2 N(0)\ln(\frac{\Delta(0)}{\Delta}) + \frac{1}{3}N(0)\pi^2 T^2 - 4N(0)T\int_0^{\omega_D}\ln(1+e^{-\sqrt{\varepsilon^2+\Delta^2}/2T})d\varepsilon \qquad (2.23)$$

When $T \to 0$, we may interpret the thermodynamic potential Ω as Gibbs free-energy density , G ,or Helmholtz free-energy density, F ,by the relation

$$G_s(T,0) = G_n(T,0) - \frac{1}{8\pi}H_c^2 \qquad (2.24)$$

and

$$F_s(T,0) = F_n(T,0) - \frac{1}{8\pi}H_c^2 \qquad (2.25)$$

H_c is the critical magnetic field of a superconductor.

As T is near 0 K, we express Eq.(2.23) in Helmholtz free-energy density's form where F_s=$F_s(T,0)$ and F_n=$F_n(T,0)$, then we get

$$F_s - F_n \cong -\frac{1}{2}N(0)\Delta^2(0) + \frac{1}{3}N(0)\pi^2 T^2 \ . \qquad (2.26)$$

Because $\int_0^{\omega_D} \ln(1+e^{-\sqrt{\varepsilon^2+\Delta^2}/T})d\varepsilon \cong 0$ and $\ln(\frac{\Delta(0)}{\Delta}) \cong 0$.

Using Eq.(2.25) and Eq.(2.26), we get

$$H_c^2 = 4\pi N(0)\Delta^2(0) - \frac{8}{3}\pi^3 N(0)T^2$$

$$= 4\pi N(0)\Delta^2(0)(1 - \frac{2}{3}\frac{\pi^2 T^2}{\Delta^2(0)})$$

or

$$H_c = H_c(0)(1 - \frac{2}{3}e^{2\gamma}(\frac{T}{T_c})^2)^{1/2} \qquad \text{, by } \frac{\Delta(0)}{T_c} = \pi e^{-\gamma}$$

$$\cong H_c(0)(1 - \frac{1}{3}e^{2\gamma}(\frac{T}{T_c})^2)$$

$$\cong H_c(0)[1 - 1.06(\frac{T}{T_c})^2] \qquad (2.27)$$

where

$$H_c(0) = \Delta(0)\sqrt{4\pi N(0)} \qquad (2.28)$$

is the critical magnetic field of superconductor at 0 K. Since N(0) determines the normal-state specific heat

$$C_n = \frac{2\pi^2}{3}N(0)k_B^2 T$$

Eqs.(2.26) and (2.28) together predict a second universal constant

$$\frac{T_c C_n(T_c)}{H_c^2(0)} = \frac{\exp(2\gamma)}{6\pi} \approx 0.168 \qquad (2.29)$$

which is independent of the material. Each of these parameters is measurable, and experimental confirmation is satisfactory in conventional superconductors.

Consider the thermodynamic potential of superconducting state, Ω_s, we have

$$\Omega_n(T)-\Omega_n(0)=-4N(0)VT\int_0^{\infty}d\varepsilon\ln(1+e^{-\varepsilon/T})=\frac{1}{3}N(0)V\pi^2T^2 \qquad (2.30)$$

and the relation of $\frac{\Omega_s-\Omega n}{v}$ at temperature T and 0 K by Eq.(2.23). Substitution from Eq.(2.30) into Eq.(2.23), we get

$$\frac{\Omega_s}{v}=\frac{\Omega_n(0)}{v}-\frac{1}{2}N(0)\Delta^2-\Delta^2N(0)\ln(\frac{\Delta(0)}{\Delta})-4N(0)T\int_0^{\omega_D}d\varepsilon\ln(1+e^{-\sqrt{\varepsilon^2+\Delta^2}/T})$$

(2.31)

When T is almost 0 K , we can use the approximation $\omega_D/T_c\rightarrow\infty$ and $\Delta\cong\Delta(0)$ and

$$\int_0^{\infty}d\varepsilon\ln(1+e^{-\sqrt{\varepsilon^2+\Delta^2}/T})\cong\frac{1}{2}e^{-\Delta(0)/T}\sqrt{2\pi T\Delta(0)}\ .$$

Substitution this relation into Eq.(2.31), then we have

$$\frac{\Omega_s}{v}\cong\frac{\Omega_n(0)}{v}-\frac{1}{2}N(0)\Delta^2(0)-2N(0)e^{-\Delta(0)/T}\sqrt{2\pi\Delta(0)T^3} \qquad (2.32)$$

Since the entropy $s=-\frac{\partial\Omega}{\partial T}$ and specific heat $c=T\frac{\partial s}{\partial T}$

then

$$\frac{s_s}{v}=2N(0)\sqrt{2\pi\Delta(0)}\ e^{-\Delta(0)/T}(\frac{3}{2}\sqrt{T}+\frac{\Delta(0)}{\sqrt{T}})$$

$$\cong 2N(0)\sqrt{\frac{2\pi}{T}}(\Delta(0))^{3/2}e^{-\Delta(0)/T}$$

and

$$\frac{c_s}{v}=2TN(0)(\Delta(0))^{3/2}\sqrt{2\pi}\ e^{-\Delta(0)/T}[-\frac{1}{2T^{3/2}}+\frac{\Delta(0)}{T^{5/2}}]$$

$$\cong 2N(0)\sqrt{2\pi}(\frac{\Delta^5(0)}{T^3})^{1/2}e^{-\Delta(0)/T} \qquad (2.33)$$

The electronic specific heat in the superconducting state obtain by Eq. (2.33) , and we find that, $c_s \ \alpha \ e^{-\Delta(0)/T}$.

In the preceding calculations we considered only the low-temperature behavior, where Δ-Δ_0 is exponentially small. Although a general evaluation of Eq.(2.17) for all $T<T_c$ requires a numerical analysis, it is possible to derive explicit expressions near T_c where $\Delta< k_B T$ provides a small parameter. We start from the gap equation Eq.(2.17) which may be expanded in powers of Δ :

$$\frac{1}{V} = 2N(0)T\int_0^{\omega_D} d\varepsilon \sum_n \frac{1}{\varepsilon^2+\Delta^2+\omega_n^2}$$

$$\cong 2N(0)T\int_0^{\omega_D} d\varepsilon \sum_n \left(\frac{1}{\varepsilon^2+\omega_n^2} - \frac{\Delta^2}{(\varepsilon^2+\omega_n^2)^2}\right)$$

We have $$\frac{d}{d\Delta}\left(\frac{1}{V}\right) \cong 4N(0)T\int_0^{\omega_D} d\varepsilon \sum_n \frac{\Delta}{(\varepsilon^2+\omega_n^2)^2}$$

then $$\frac{\Omega_s-\Omega_n}{v} = -4N(0)T\int_0^{\omega_D} d\varepsilon \sum_n \int_0^{\Delta} d\Delta' \frac{\Delta'^3}{(\varepsilon^2+\omega_n{}^2)^2}$$

$$= -N(0)T\Delta^4\int_0^{\omega_D} d\varepsilon \sum_n \frac{1}{(\varepsilon^2+\omega_n^2)^2}$$

Using the approximation $\omega_D >> T_c$ then $\int_0^{\omega_D} \to \int_0^{\infty}$.

We have $$\int_{-\infty}^{\infty} \frac{1}{(\varepsilon^2+\omega_n^2)^2} d\varepsilon = \frac{\pi}{2\omega_n^3}$$

Above equation yields

$$\frac{\Omega_s-\Omega_n}{v} = -N(0)T\Delta^4 \sum_{n=-\infty}^{\infty} \frac{\pi}{4}\cdot\frac{1}{\omega_n^3}$$

$$= -\frac{N(0)\Delta^4}{2\pi^2 T^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^3}$$

$$= -\frac{7}{8}\zeta(3)N(0)\frac{\Delta^4}{2\pi^2 T_c^2} \qquad ,T \to T_c\ .$$

Substituting Δ^2 from Eq.(2.26) into the above equation, we have

$$\frac{\Omega_s-\Omega_n}{v} = -\frac{7}{8}\zeta(3)\frac{N(0)}{2\pi^2 T_c^2}\left(\frac{8}{7\zeta(3)}\right)^2 \pi^4 T_c^2 (T_c - T)^2$$

$$= -\frac{8}{7\zeta(3)} N(0) \frac{\pi^2 T_c^2}{2} (1 - \frac{T}{T_c})^2 \qquad (2.34)$$

Changing the thermodynamic potential to be Helmholtz free-energy density by the relation

$$\frac{\Omega_s - \Omega_n}{v} = F_s - F_n = -\frac{1}{8\pi} H_c^2$$

where $H_c(0) = \sqrt{4\pi N(0)}\, \Delta(0) = \sqrt{4\pi N(0)}\, \pi e^{-\gamma} T_c$.

We can rewrite Eq.(2.34) as

$$H_c = H_c(0) e^{\gamma} [\frac{8}{7\zeta(3)}]^{1/2} (1 - \frac{T}{T_c})$$

$$\cong 1.74\, H_c(0)(1 - \frac{T}{T_c}) \qquad , T \to T_c \quad . \qquad (2.35)$$

Eqs.(2.27) and (2.35) are very similar to the phenomenological relation.

We also have the relation between the Helmholtz free-energy density and the magnetic field at temperature T , T<T_c , as

$$F_s(T,H) - F_n(T,H) = \frac{1}{8\pi}(H^2 - H_c^2) \qquad (2.36)$$

We have $s = -(\frac{\partial F}{\partial T})$, s-entropy, and H_c=$H_c(T)$ then

$$s_s(T,H) - s_n(T,H) = \frac{1}{4\pi} H_c(T) \frac{d}{dT} H_c(T)$$

and the specific heat is given by $c = T(\frac{\partial s}{\partial T})$.

We obtain

$$c_s - c_n = \frac{T}{4\pi}[(\frac{dH_c}{dT})^2 + H_c \frac{d^2}{dT^2} H_c(T)]$$

At $T=T_c$,

$$c_s - c_n = \frac{T_c}{4\pi}\left(\frac{dH_c}{dT}\right)^2\Big|_{T=T_c}$$

where H_c is defined by Eq.(2.35), so we find

$$\frac{dH_c}{dT} = -\frac{H_c(0)e^{\gamma}}{T_c}\left(\frac{8}{7\zeta(3)}\right)^{1/2} = \pi\sqrt{4\pi N(0)}\left(\frac{8}{7\zeta(3)}\right)^{1/2}$$

Let $c_n = (2/3)\pi^2 N(0)T$ is normal state specific heat then we get

$$\frac{c_s - c_n}{c_n}\Big|_{T=T_c} = \frac{12}{7\zeta(3)} \cong 1.43 \qquad (2.37)$$

which is in a perfect agreement with the experimental results for a conventional superconductor as shown in Table(2.1).

Element	T_c(K)	$\frac{c_s - c_n}{c_n}\Big\vert_{T=T_c}$
Al	1.16	1.45
Zn	0.85	1.27
Ga	1.08	1.44
In	3.4	1.73
Tl	2.38	1.5
V	5.3	1.49
Pb	7.19	2.71
Nb	9.22	1.87

Table(2.1) Data relevant to the specific heat jumps at T_c for some elemental superconductors (Burns, 1992).

Isotope Effect

We define the the definition of isotope exponent , α, as

$$\alpha = -\frac{\partial \ln T_c}{\partial \ln M} \qquad (2.38)$$

where M is the atomic mass. If atom motions behave harmonically, the Debye frequency will be proportional to $1/\sqrt{M}$ as

$$\omega_D \alpha \frac{1}{\sqrt{M}} \quad .$$

With this condition, the isotope exponent can be written in the following form.

$$\alpha = \frac{1}{2}\frac{\partial \ln T_c}{\partial \ln \omega_D}$$

$$= \frac{1}{2}\frac{\omega_D}{T_c}\frac{\partial T_c}{\partial \omega_D} \qquad (2.39)$$

From the Eq.(2.13), the derivative of T_c respect to ω_D is

$$\frac{\partial T_c}{\partial \omega_D} = \frac{T_c}{\omega_D} \qquad (2.40)$$

Substituting Eq.(2.39) in Eq.(2.40), we get

$$\alpha = \frac{1}{2} \qquad (2.41)$$

The BCS isotope exponent of a superconductor under an harmonic approximation is equal to 1/2 .

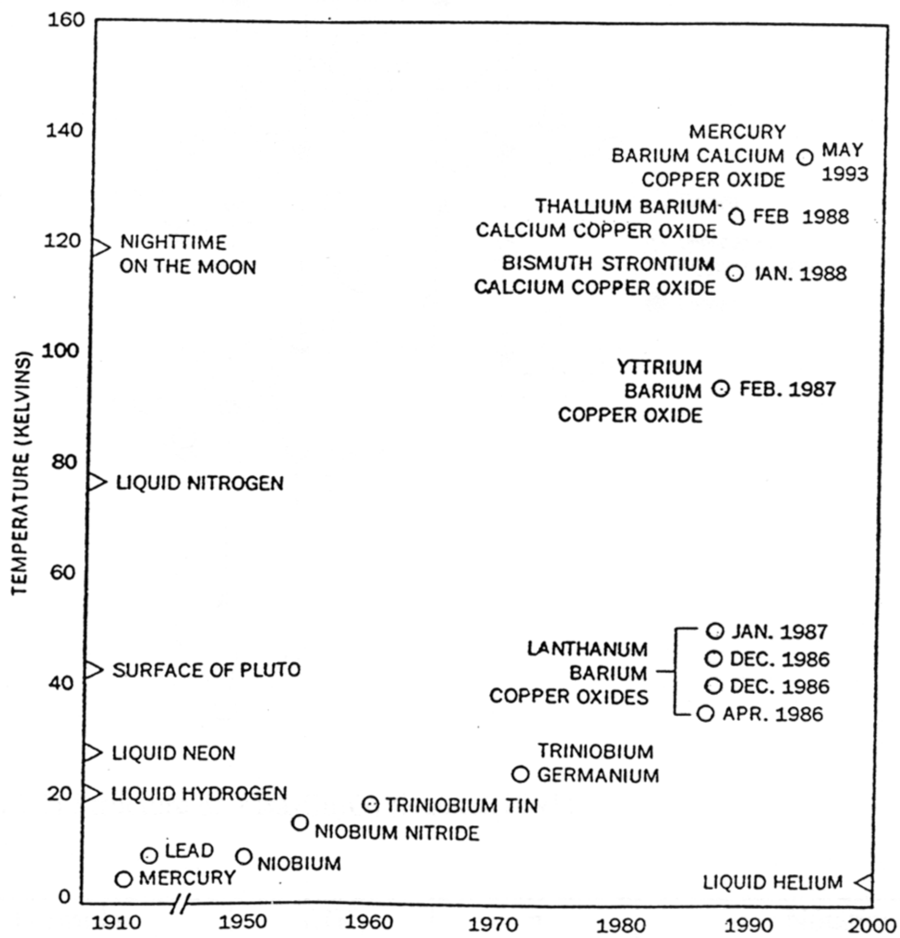
CHAPTER III

HIGH-T_c SUPERCONDUCTOR

The Discovery of High-T_c Superconductor

The first of a new family of superconductors, now usually known as the high-T_c or cuprate superconductors, was discovered in 1986 by Bednorz and Muller (1986). It was a calcium-doped lanthanum cuprate perovskite. When optimally doped to give the highest T_c, it had the formula $La_{1.85}\,Ca_{0.15}\,CuO_4$, with a T_c of 30 K. This was already sufficiently high to suggest to the superconductivity community that it might be difficult to explain using the usual forms of BCS theory, and a large number of related discoveries followed quickly. In the following year Wu et al. (1987) found that the closely related material $YBa_2Cu_3O_{7-\delta}$, now known as “1,2,3 compound”, has a T_c of about 93 K when δ=0.10 , well above the boiling point of liquid nitrogen (T=77 K) . With superconductivity at temperatures above the the boiling point of liquid nitrogen it was possible to enthuse about the large-scale industrial application of this phenomenon.

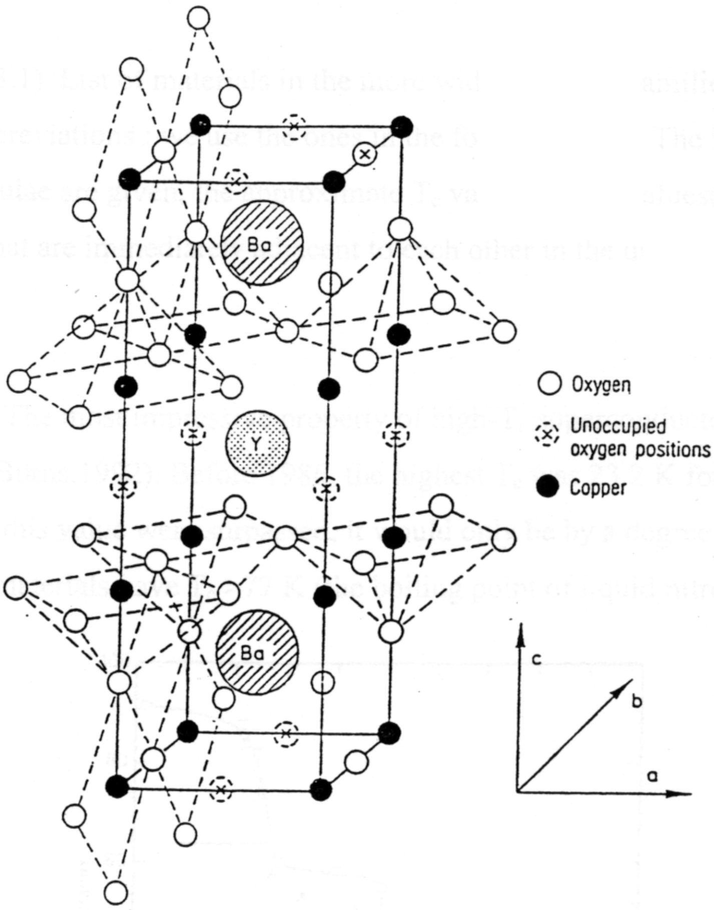
Within the space of one year (1987) the properties of the new materials were studied very precisely and the results published in a large number of papers. In 1988, there were reports of new superconductors in systems Bi-Sr-Ca-Cu-O (Maeda et al., 1988) with T_c values of up to 110 K and in Tl-Ba-Ca-Cu-O with T_c values of over 120 K (Parkin et al., 1988) .



Figure(3.1) Sharply rising critical temperature in superconductors stem from the cuprate materials (Kirtley and Tsuei ,1996).

Structures

Compared to structures encountered in most areas of solid-state physics, those of the high-T_c crystals are complicated.They are layer compounds typically tetragonal, or orthorhombic and close to tetragonal, and contain Cu-O planes with the formula CuO_2 lying normal to the c direction. These planes contain mobile charge carriers and are thought to be seat of the superconductivity. The carriers are usually sharply localized in the planes, and this makes contact between the planes relatively weak. For this reason the cuprates often have extremely anisotropic properties.



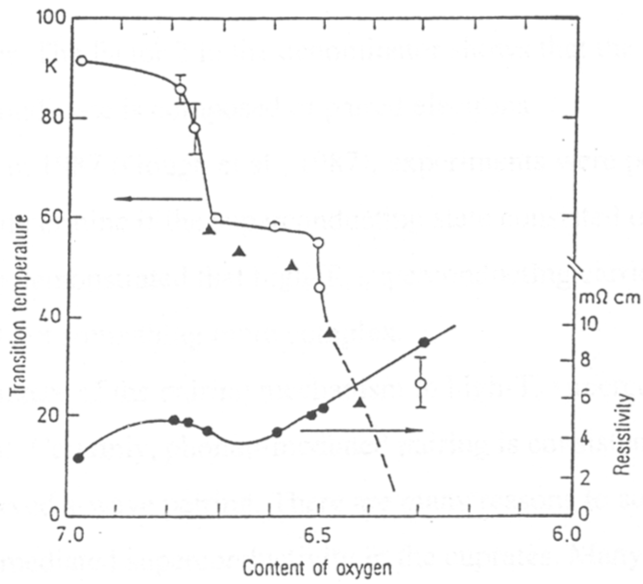
Figure(3.2) Structure of $YBa_2Cu_3O_7$ (Buckel,1991).

Formula	T_c(K)	n	Notation	
$(La_{2-x}Sr_x)CuO_4$	38	1	La(n=1)	214
$(La_{2-x}Sr_x)CaCu_2O_6$	60	2	La(n=2)	-
$Tl_2Ba_2CuO_6$	0-80	1	2-Tl(n=1)	Tl2201
$Tl_2Ba_2CaCu_2O_6$	108	2	2-Tl(n=2)	Tl2212
$Tl_2Ba_2Ca_2Cu_3O_{10}$	125	3	2-Tl(n=3)	Tl2223
$Bi_2Sr_2CuO_6$	0-20	1	2-Bi(n=1)	Bi2201
$Bi_2Sr_2CaCu_2O_8$	85	2	2-Bi(n=2)	Bi2212
$Bi_2Sr_2Ca_2Cu_3O_{10}$	110	3	2-Bi(n=3)	Bi2223
$YBa_2Cu_3O_7$	92	2	Y123	YBCO
$YBa_2Cu_4O_8$	80	2	Y124	-
$Y_2Ba_4Cu_7O_{14}$	40	2	Y247	-

Table(3.1) List of materials in the more widely studied families along with descriptive abbreviations : we use the ones in the fourth column. The idealized chemical formulae are given, the approximate T_c values, and n values(n refer to the n Cu-O planes that are immediately adjacent to each other in the unit cell)(Burns,1992).

T_c values

The most impressive property of high-T_c superconductors is their high values of T_c (Burns,1992). Before 1986, the highest T_c was 23.2 K for Nb_3Ge, and it was felt that if this value were surpassed, it would only be by a degree or two. Now many high-T_c materials have T_c >77 K (the boiling point of liquid nitrogen), as shown in Figure(3.1).



Figure(3.3) Influence of the oxygen content on the critical temperature T_c and the electrical resistivity of $YBa_2Cu_3O_{7-\delta}$: ooo, • • • (Batlogg et al., 1987); ▲▲▲ (Tarascon et al., 1987).

The effect of doping on T_c for all of the high-T_c materials is the same manner as shown in case of $YBa_2Cu_3O_{7-\delta}$. For $YBa_2Cu_3O_{7-\delta}$, the variation of T_c with doping is shown in Figure(3.3). This can be done by subjugating the crystals to excess oxygen pressure or a reducing atmosphere. Or the doping can be changed by replacing some of the Y^{3+} by Ca^{2+} ; both of these ions usually occupy positions between the immediately adjacent Cu-O planes. T_c vs. doping (carrier concentration) curve for the most of high-T_c materials is bell-shaped curve. There appears to be optimal doping for the highest T_c. Also, most of these materials can be doped until they become insulators or non-superconducting metals.

Paired Electron (Burns,1992)

In conventional superconductors, by measuring the magnetic flux,ϕ, trapped in hollow superconducting cylinders, It was found that this flux is an integral multiple of a fundamental unit, the fluxoid quantum ϕ_0 such that

$$\phi = n(h / 2e) = n\phi_0$$

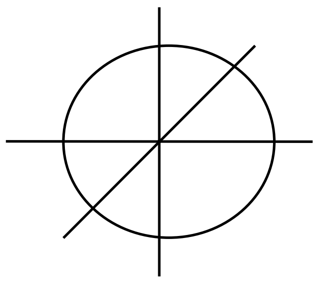
where n is any integer. The factor 2 in the denominator shows that the superconducting ground state is composed of paired electrons.

Early in 1987 (Gough et al., 1987), experiments were performed on high-T_c materials to determine if the superconducting state consisted of paired electrons. It has been demonstrated that high-T_c superconducting carriers consist of paired electrons, and not some thing more complex.

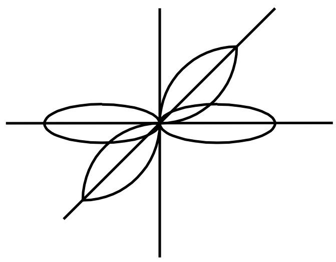
The nature of the pairing mechanism in high-T_c superconductors is not understood at present. Certainly, phonon-mediated pairing is consistent with the experimentally observed s-wave pairing. There are many reasons to support and not support the phonon-mediated superconductivity in the cuprates. Many non-phonon pairing mechanisms have been suggested for the high-T_c materials. Spin-fluctuation exchange mechanisms or mechanisms based on large on-site Coulomb repulsion tend to give d- or p-state pairing, but much more work remain to be done.

Evidence of Non-S-Wave Pairing

The cooper pairs of conventional superconductors take on s-wave symmetry. This is the chance of finding one carrier in a Cooper pair given the position of the other falls off at the same rate in all direction in space. If we plot the wave function keeping one member of the Cooper pair at the center, the probability of finding its partner would appear as a sphere around the center. The next most highly symmetric state for the cuprates is the d state. Plotted, it would appear as four lobes lying in plane, like a four-leaf clover. Each lobe represents a likely position of one member of the Cooper pair with respect to its partner. D symmetry also means that the Cooper pair members are not so close to each other that their mutual repulsion interferes with their coupling (Kirtley and Tsuei,1996).



s-wave symmetry



d-wave symmetry

Figure(3.4)Two types of symmetry of the superconducting wave function are s-wave and d-wave. In the s-wave condition, one member of a Cooper pair is located in the spherical area around its partner. For d-wave symmetry, the partner lies somewhere in one of the four lobes (Kirtley and Tsuei ,1996).

In s-wave states, Δ_k may be taken to be real and without nodes. The gap then has the full crystal symmetry and only relative weak anisotropy. In d-wave superconductivity, the gap have the same symmetry as an x^2-y^2 orbital with nodes at 45^o to the a and b axes if we have full tetragonal symmetry (Figure(3.2)). For an orthorhombic symmetry the corresponding state will be somewhat distorted, with the nodes no longer at exactly 45^o (Annett et al., 1990) .

Evidence which is more specific comes from Josephson effect experiments of Kirtley and Tsuei (1996) that have shown that the yttrium-based and bismuth-based superconductors are all consistent with d-wave symmetry.

In case of cubic lattice, Scalapino, Loh and Hirsch (1987) find the different types of wave function of Cooper pairs as

$$\Psi_s(p) = 1 \qquad \text{for s-wave}$$

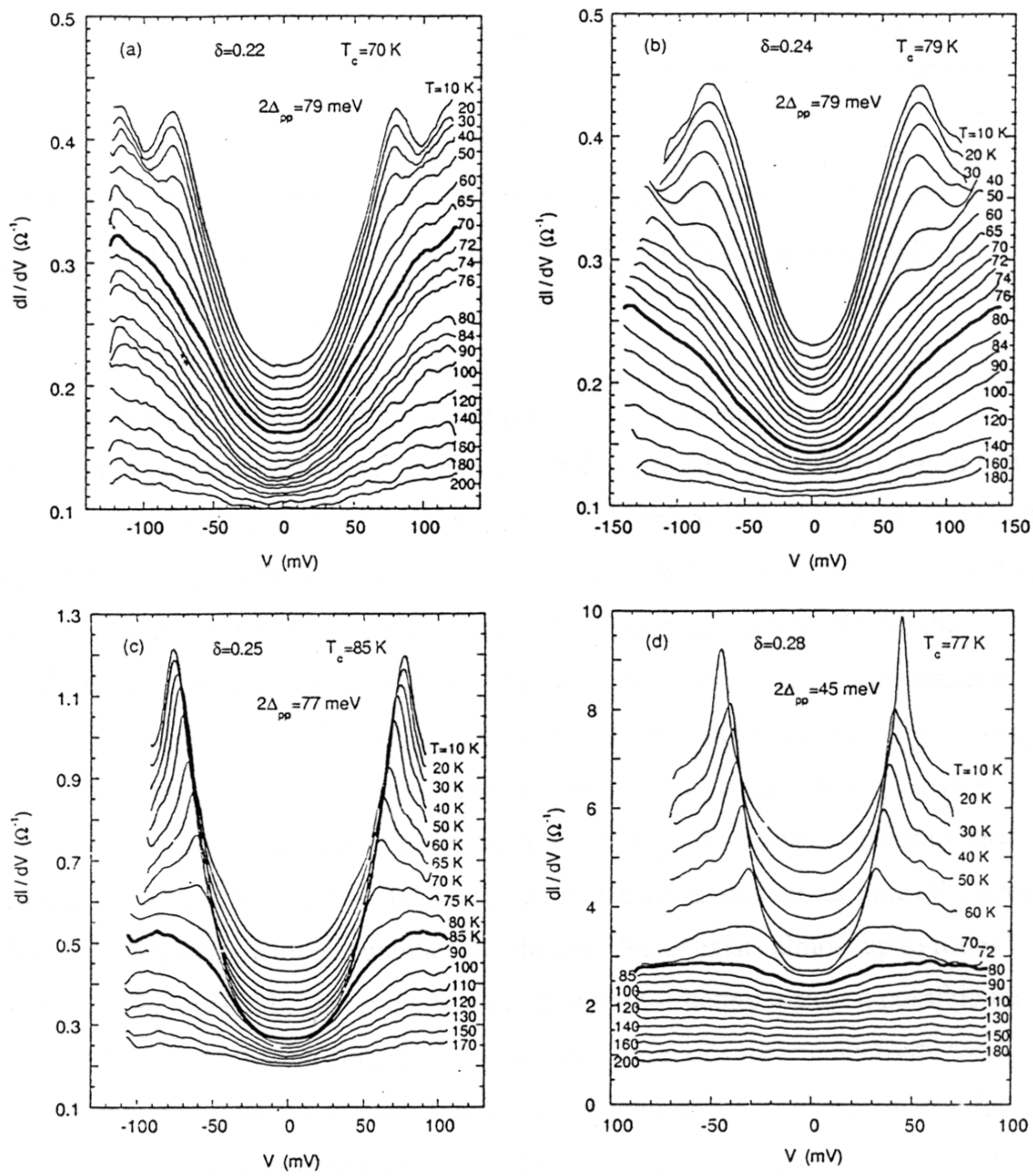
$$\Psi_{d_{x^2-y^2}}(p) = \cos p_x a - \cos p_y a \qquad \text{for d-wave}$$

If we ignore the lattice effect then $\Psi_{d_{x^2-y^2}}(p) = \cos 2\theta_p$ which corresponds to a gap function $\Delta(p) = \Delta(T)\cos 2\theta_p$ where θ_p is the polar angle in the plane (Fehrenbacher and Norman, 1994).

Pseudogap

The existence of a pseudogap (PG) in the normal state of underdoped in high-T_c superconductors is considered to be among the most important features of cuprates. Evidence for gaplike structure in the normal state at $T^* > T_c$ was provided by variety of experimental methods, particularly by angle-resolved photoemission spectroscopy (ARPES) measurements in $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Ding et al., 1996), nuclear magnetic resonance (NMR) and nuclear quadrupole resonance (NQR) results in $YBa_2Cu_4O_8$ (Williams et al., 1998; Raffa et al., 1998) and neutron spectroscopic measurements in $Tm_{0.1}$ $Y_{0.9}$ $Ba_2Cu_3O_{6.9}$ (Osborn and Goremychkin, 1991), $HoBa_2Cu_4O_8$ and $Er_2Ba_4Cu_7O_{15}$ (Mesot et al., 1998; Rubio et al., 2000).

The remarkable properties of PG are discussed by many researchers, some of them are shown below. Ding et al.(1996) find that a pseudogap with d-wave symmetry opens up in the normal state below T* and develops into the d-wave superconducting gap below T_c. Kristoffel and Ord (1998)show that this pseudogap is related to the superconducting gap (order parameter) below T_c and acts as a normal-state precursor of the true gap. The pseudogap seems to be a property of underdoped high-T_c materials becoming suppressed in the optimally doped region. Renner (1998) suggested that superconducting gap (SG) smoothly connects with pseudogap at T_c with a sizable magnitude. Bouvier and Bok (2000) suggest that the pseudogap is only seen in the underdoped sample. The pseudogap has not been observed in the conventional superconductors. The pseudogap magnitude decreases with doping with anisotropic in the CuO_2 planes and PG have the same symmetry as SG. Suzuki and Watanabe (2000) find that PG magnitude ($T=T_c$) is much greater than SG (T=0 K) in the underdoped region but PG magnitude is much smaller than SG in the overdoping region. Both gaps show the smooth connection near the optimum doping.



Figure(3.5) dI/dV-V curves at various temperature for the specimens in $Bi_2Sr_2CaCu_2O_{8+\delta}$ system. The thick lines indicate curve very close to T_c (Suzuki and Watanabe, 2000).

T_c (K)	SG at T=0 K, (K)	PG at T_c, (K)
70	457.9	869.5
79	457.9	753.6
85	446.3	463.7
77	260.8	173.9

Table(3.2). Shows the magnitude of superconducting gap (SG) at T=0 K and pseudogap (PG) at T=T_c for different T_c in $Bi_2Sr_2CaCu_2O_{8+\delta}$ system (Suzuki and Watanabe, 2000) .

The explanation for origin of the pseudogap is not clear yet but many proposals have been presented. Fukuyama (1992) and Lee et al.(1998) suggest that the pseudogap is caused by the singlet formation of spinons which appears as a result of the spin-charge separation. Emery and Kivelson (1995), Kwon and Dorsey (1999), and Koikegami and Yamada (2000) suggest that pseudogap is related with the antiferromagnetic phase which is reached by controlling the doping or the pressure.

The most accepted theory is proposed by Emery and Kivelson (1995) . They pointed out that superconductivity requires more than just paired charge carriers, it also requires" phase coherence" between those pairs.Each pair has a quantum wave associated with it, for the pairs to condense into the superconducting state all waves have to be in phase with one another. As the pseudogap exists almost up to room temperature, it could be that some feature of cuprate structure makes it possible for pairs to form at high temperature above T_c. If the onset of superconductivity would signify not the formation of pairs, but the setting in of phase coherence below T_c . This idea is supported from experiments by Corson et al.,(1999) in $Bi_2Sr_2CaCu_2O_{8+\delta}$. They found exactly the sort of fluctuations above T_c . In Emery and Kivelson theory, above T_c the pairs have so much thermal energy that they can no longer maintain phase coherence. Superconductivity should become fragmented or fluctuating.

Comment on High-T_c Superconductor

Knowledge of mechanism of pairing of carriers and of the nature of the normal state is central to an understanding of the high-T_c superconductors. Superconductivity is a correlated many body state of pairs which is well described by the BCS theory in weak-coupling limit $\lambda<1$. Depending on the specific bosonic field, which glues two carriers together, the BCS superconductor could be not only phononic but also excitonic, and plasmonic .

The BCS theory like any mean-field theory is a rather universal description of the cooperative-quantum phenomenon of superfluidity in ^{3}He with T_c a few mK, in a conventional superconductor, and as is believed, even in atomic nuclei with $T_c = 10^{10}$ K (Anderson and Schrieffer, 1991).

We will compare the properties of the high-T_c materials to the results of BCS . In BCS theory it is assumed that the attractive electron-pairing interaction is due to electron-phonon coupling, that pair are weakly coupled compared to average phonon energies (call weak-coupled BCS), and that pair are in a spin-singlet s-state which implies that the superconducting energy gap is isotropic. In the high-T_c superconductors, they show many unusual effects.

In some observations, they find that the high-T_c superconductors are almost identical to conventional BCS superconductor's properties. But in some observations , there are still difficult to reconcile their unusual properties to BCS .We list a few of these here (Burns,1992).

1. In the superconducting state, the electron are paired. Although theses materials show electron-pairing superconductivity, it is possible that the pairing interaction may not be phonon-mediated. Phonon-mediated superconductivity with some sort of a booster to increase T_c is also a possibility.

2. There is an energy gap in the superconducting state as in conventional superconductors. However, the energy gap is probably anisotropic and lies in the range 3.5 to 8 k_BT_c, which is larger than the isotropic BCS value of 3.54 .

3. Several experiments suggest pairing into s-wave state, as predicted by BCS. But there are several experiments shown d-wave state in high-T_c superconductor.

4. The high-T_c materials display many of the familiar superconducting properties, such as Josephson tunneling and vortex structure as found in BCS superconductors.

At this state, we think that BCS theory can describe properties of high-T_c superconductor if we modify this theory by using the facts from experimental data.

CHAPTER IV

THEORETICAL SURVEY OF HIGH-T_c SUPERCONDUCTOR IN BCS SCENARIO

Van Hove Singularity Density of States

A Van Hove singularity scenario (VHS) in the electronic density of states (DOS) was initially proposed (Labbe et al., 1976 ; Kieselmann and Rietshel, 1982; Hirsch et al., 1986) to explain T_c enhancement in superconductors over and above the T_c predicted by BCS theory. Since the origin of cuprate superconductivity is to be found in CuO_2 planes, which are weakly coupled together along perpendicular axis, their electronic structures will be quasi-two-dimensional (2D). This necessarily leads to at least one VHS coinciding with saddle point in the ε(k) surface, these saddle points being present in all 2D band structures.

Getino et al.(1993) derive the exact T_c formula within the VHS scenario. They begin with the equation for the finite-temperature gap energy Δ(T), with a general density of states N(E),

$$\frac{2}{V}=\int_{E_F-\omega_D}^{E_F+\omega_D}\frac{dE}{\sqrt{(E-E_F)^2+\Delta^2(T)}}N(E)\tanh\left[\frac{\sqrt{(E-E_F)^2+\Delta^2(T)}}{2T}\right] \tag{4.1}$$

where V is a positive coupling constant representing the electron-phonon interaction, which is nonzero in a narrow shell of thickness $2\omega_D$ centered about the Fermi energy E_F . They assume a Van Hove singularity DOS of the form

$$N(E)=N_0\ln\left|\frac{E_F}{E-E_F}\right| \tag{4.2}$$

Putting $x=(E-E_F)/2T_c$, $Z=\omega_D/2T_c$, and $W=E_F/2T_c$, in Eq.(1) and Eq.(2) with $\Delta(T_c)=0$, they obtain

$$\frac{1}{N_0V}=\int_0^Z dx\frac{\tanh x}{x}\ln\frac{W}{x} \quad (4.3)$$

Integrating this by parts gives

$$\frac{1}{N_0V}=\tanh Z\ln Z\ln\frac{W}{Z}+\frac{1}{2}\tanh Z\ \ln^2 Z-D(Z,W) \quad (4.4)$$

where

$$D(Z,W)=\int_0^Z dx(\ln x\ \ln\frac{W}{x}+\frac{1}{2}\ln^2 x)\sec h^2 x \quad (4.5)$$

Multiplying both sides of Eq.(4.4) by 2 cothZ, adding $\ln^2(W/Z)$, and rearranging, leads to

$$[\frac{1}{N_0V}+D(Z,W)]2\coth Z+\ln^2\frac{W}{Z}=\ln^2 W \quad (4.6)$$

which on exponentiation leaves the exact T_c formula given by

$$T_c=\frac{1}{2}E_F\exp\left\{-[(\frac{1}{N_0V}+D(\frac{\omega_D}{2T_c},\frac{E_F}{2T_c}))2\coth\frac{\omega_D}{2T_c}+\ln^2\frac{E_F}{\omega_D}]^{1/2}\right\} \quad (4.7)$$

This T_c's equation provides significantly larger values for T_c than the standard BCS formula as shown in Table(4.1).

	N_0V	ω_D(K)	E_F(K)	T_c(K)
BCS with VHS	0.081	754	5800	40
	0.12	754	5800	92
Standard BCS	0.081	754	-	0.004
	0.12	754	-	0.2

Table(4.1) Shows the comparison of T_c between BCS and VHS (Tsuei et al., 1990) .

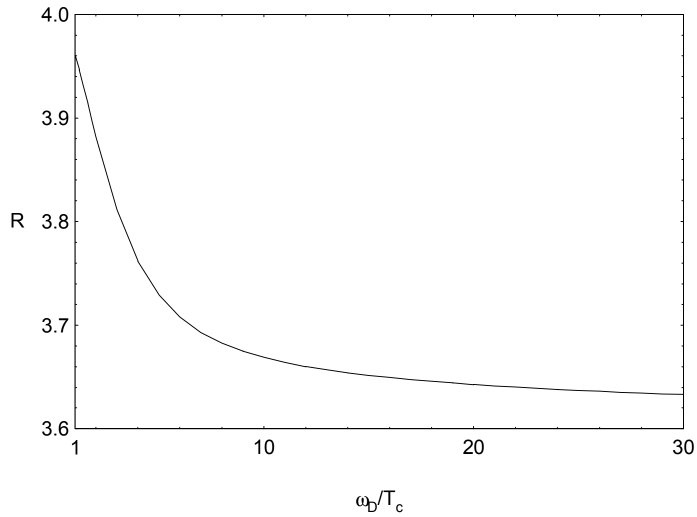
Gap-to-T_c Ratio

Getino et al.(1993) calculated the exact T_c equation, Eq.(4.7), but they evaluated gap-to-T_c ratio (R) approximately. Ratanaburi et al.(1996) derived an exact R equation as

$$\int_0^{\omega_D/2T_c} dx \frac{\tanh x}{x} \ln\left|\frac{E_F}{2xT_c}\right| = \int_0^{2\omega_D/RT_c} dx \frac{\ln\left|2E_F / RT_c x\right|}{\sqrt{x^2+1}} \qquad (4.8)$$

where $R=2\Delta_0/T_c$.

The numerical calculation of R based on Eq.(4.8) is shown in Figure(4.1) .



Figure(4.1) Value of R for a DOS with a VHS at the Fermi level for different ω_D/T_c values and taking E_F=4000 K and ω_D=500 K (Ratanaburi et al.,1996).

Figure(4.1) showed that the values of R do decrease with increase in ω_D/T_c and tend to reach the BCS limit of 3.53 for very high value of ω_D/T_c The reason for this is because the increase in ω_D/T_c enlarges the effective region of the DOS and hence the R value is diminished.

At this step, we derive Eq.(4.8) for an exact solution of R and get

$$\int_0^{\omega_D/2T_c} dx \frac{\tanh x}{x} \ln\left|\frac{E_F}{2T_c x}\right| = 2\sum_{n=0}^{\infty} \frac{1}{\pi(n+1/2)}[\ \tan^{-1}(\frac{\omega_D}{2\pi T_c(n+1/2)}) \ln(\frac{E_F}{2\pi T_c(n+1/2)})$$

$$+ Cl_2(2\tan^{-1}(\frac{\omega_D}{2\pi T_c(n+1/2)})) - \frac{1}{4} Cl_2(4\tan^{-1}(\frac{\omega_D}{2\pi T_c(n+1/2)}))\ ]$$

and

$$\int_0^{2\omega_D/RT_c} dx \frac{\ln(\frac{2E_F}{RT_c})}{\sqrt{x^2+1}} = \sinh^{-1}(\frac{2\omega_D}{RT_c}) \ln(\frac{4E_F}{RT_c}) + \mathrm{Re}[\frac{1}{2i} Cl_2(2i \sinh^{-1}(\frac{2\omega_D}{RT_c}))] \quad .$$

where $Cl_2(z) = -\int_0^z dx \ln(2\sin(\frac{x}{2}))$ is the Clausen integral (Prudnikov, Brychkov, and Marichev, 1992).

Combining the above equations, we get

$$R = \frac{4E_F}{T_c} \exp[\frac{-1}{\sinh^{-1}(\frac{2\omega_D}{RT_c})} \{2\sum_{n=0}^{\infty} \frac{1}{\pi(n+1/2)}[\ \tan^{-1}(\frac{\omega_D}{2\pi T_c(n+1/2)}) \ln(\frac{E_F}{2\pi T_c(n+1/2)})$$

$$+ Cl_2(2\tan^{-1}(\frac{\omega_D}{2\pi T_c(n+1/2)})) - \frac{1}{4} Cl_2(4\tan^{-1}(\frac{\omega_D}{2\pi T_c(n+1/2)}))\ ]$$

$$- \mathrm{Re}[\frac{1}{2i} Cl_2(2i \sinh^{-1}(\frac{2\omega_D}{RT_c}))]\}\ ] \qquad (4.9)$$

Isotope Effect

In harmonic approximation

$$\alpha = \frac{1}{2} \frac{\omega_D}{T_c} \frac{dT_c}{d\omega_D} \qquad (4.10)$$

Rewrite Eq.(4.3) as

$$\frac{1}{N_0 V} = \int_0^{\omega_D/2T_c} \frac{dx}{x} \ln(\frac{E_F}{2T_c x}) \tanh x \qquad (4.11)$$

Differentiation Eq.(4.11) with respect to ω_D all the way, we find

$$\frac{\partial T_c}{\partial \omega_D} = \frac{T_c}{\omega_D} \frac{\ln(\frac{E_F}{\omega_D}) \tanh(\frac{\omega_D}{2T_c})}{\ln(\frac{E_F}{\omega_D}) \tanh(\frac{\omega_D}{2T_c}) + \int_0^{\omega_D/2T_c} \frac{dx}{x} \tanh x} \qquad (4.12)$$

Since

$$\int_0^{\omega_D/2T_c} \frac{dx}{x}\tanh x = \sum_{n=0}^{\infty}\int_0^{\omega_D/2T_c} dx \frac{2}{x^2+(\pi(n+\frac{1}{2}))^2}$$

$$= \sum_{n=0}^{\infty}\frac{2}{\pi(n+\frac{1}{2})}\tan^{-1}\left(\frac{\omega_D}{2\pi T_c(n+\frac{1}{2})}\right)$$

Substituting Eq.(4.12) into Eq.(4.10), we get

$$\alpha = \frac{1}{2}\frac{\ln(\frac{E_F}{\omega_D})\tanh(\frac{\omega_D}{2T_c})}{[\ln(\frac{E_F}{\omega_D})\tanh(\frac{\omega_D}{2T_c}) + \sum_{n=0}^{\infty}\frac{2}{\pi(n+\frac{1}{2})}\tan^{-1}(\frac{\omega_D}{2\pi T_c(n+\frac{1}{2})})]} \tag{4.13}$$

Asymmetry of the Isotope Exponent

Tsuei et al.(1990) and Goicochea(1994) used a VHS model to explain the dependence of α on doping superconductor. They showed that a maximum transition temperature with minimum isotope shift exponent occurs when the Fermi level lies at the energy of the VHS, and T_c decreases while α increases as the Fermi level is displaced from the VHS. This behavior is in good agreement with the experimental results of high-T_c oxide systems. Apart from exhibiting a minimum at optimum doping, the α curve is asymmetric about the point where T_c is maximum. Bhardwaj and Muthu (2000) have used a slightly modified version of a VHS to explain the asymmetry in the α curve. They consider a DOS with a Van Hove singularity of the form

$$N(E) = N_0\left|\frac{E_F}{E-E_F-\delta}\right| \tag{4.14}$$

where $\delta = -\delta_1 : E_F-\omega_D \leq E \leq E_F$

$= \delta_2 : \quad E_F \leq E \leq E_F + \omega_D$

and $0 \leq \delta_2, \delta_2 \leq 2T_c$.

Using Eq.(4.1) and taking $T=T_c$ ($\Delta(T_c)=0$), the BCS gap equation is

$$\frac{2}{N_0 V} = \int_{E_F-\omega_D}^{E_F+\omega_D} dE \frac{\tanh(\frac{E-E_F}{2T_c})}{E-E_F} \ln\left|\frac{E_F}{E-E_F-\delta}\right|$$

$$= I_1 + I_2 \tag{4.15}$$

with $I_1 = \int_0^{\omega_D} \frac{dx}{x} \tanh(\frac{x}{2T_c}) \ln\left|\frac{E_F}{x-\delta_1}\right|$ and

$$I_2 = \int_0^{\omega_D} \frac{dx}{x} \tanh(\frac{x}{2T_c}) \ln\left|\frac{E_F}{x-\delta_2}\right| \tag{4.16}$$

Bhardwaj and Muthu (2000) have made an approximate calculation of the α exponent but here we can work out the equation to get the exact solution for α defined by Eq.(4.10) . First, we separate the limit of integration into 2 parts

$$I = \int_0^{\delta} \frac{dx}{x} \tanh(\frac{x}{2T_c}) \ln(\frac{E_F}{\delta - x}) + \int_{\delta}^{\omega_D} \frac{dx}{x} \tanh(\frac{x}{2T_c}) \ln(\frac{E_F}{x-\delta})$$

Differentiating Eq.(4.15) with respect to ω_D all the way, we find

$$\alpha = \frac{\frac{1}{2}\tanh(\frac{\omega_D}{2T_c}) \ln(\frac{E_F^2}{(\omega_D-\delta_1)(\omega_D-\delta_2)})}{\tanh(\frac{\omega_D}{2T_c}) \ln(\frac{E_F^2}{(\omega_D-\delta_1)(\omega_D-\delta_2)}) - T_c(f(\delta_1)+f(\delta_2))} \tag{4.17}$$

where

$$f(\delta) = \frac{1}{T_c}\tanh(\frac{\delta}{2T_c}) \ln(\frac{\delta}{\omega_D - \delta})$$
$$+\sum_{n=0}^{\infty} (\frac{2}{\delta^2 + (\pi T_c(2n+1))^2})[\delta \ln[(\frac{\omega_D}{2T_c})^2 + (\pi(n+1/2))^2] - 2\delta\ln(\pi(n+1/2))$$
$$-2\pi T_c(2n+1)\tan^{-1}(\frac{\omega_D}{\pi T_c(2n+1)})\ ]$$

For $\delta = \delta_1 = -\delta_2$, the density of state can be reduced to be

$N(\varepsilon) = N_0 \ln\left|\frac{E_F}{\varepsilon - (E_F - \delta)}\right|$ that is considered by Goicochea (1994). We can get

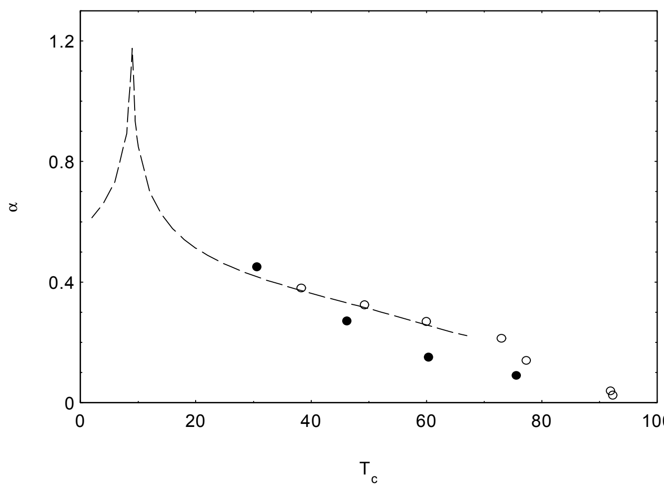
$$\alpha = \frac{1}{2}\frac{\tanh(\frac{\omega_D}{2T_c})\ln(\frac{E_F^2}{\omega_D^2-\delta^2})}{\{\tanh(\frac{\omega_D}{2T_c})\ln(\frac{E_F^2}{\omega_D^2-\delta^2})+\tanh(\frac{\delta}{2T_c})\ln(\frac{\omega_D-\delta}{\omega_D+\delta}) + 4\sum_{n=0}^{\infty}\frac{2\pi(n+1/2)\tan^{-1}(\omega_D/\pi T_c(2n+1))}{(\frac{\delta}{2T_c})^2+(\pi(n+1/2))^2}\}}$$

(4.18)

Goicochea (1994) derived the T_c formula which corresponds to the density of states, $N(\varepsilon)=N_0\ln\left|\frac{E_F}{\varepsilon-(E_F-\delta)}\right|$, as

$$T_c = 1.36E_F\exp\{-[\frac{2}{N_0V}+\ln^2(\frac{E_F}{\omega_D})+\frac{\delta^2}{2}(\frac{1}{(2T_c)^2}+\frac{1}{\omega_D^2})-1]^{1/2}\} \qquad (4.19)$$

Using Eq.(4.15)-(4.19), we can get the numerical result of α, for case $\delta=\delta_1=-\delta_2$,as shown in Figure(4.2).



Figure(4.2) Isotope effect exponent (α) as a function of T_c. Here we have used E_F=500 meV, ω_D=65 meV, and NV_0 = 0.11. Experimental data are taken from Franck et al. (1991)(ooo) and Bornemann and Morris (1991) (• • •) (Goicochea ,1994).

Figure(4.2) shows the isotope exponent as a function of T_c for a VHS , and the results are compared to experiments on the yttrium-based compounds. The lowest value of the isotope exponent remain unattainable with a VHS.

Power Law Density of States

Because of the high value of R above the BCS result, it is possible to take into account of any DOS singularity. Mattis and Molina (1991) evaluated the zero-temperature gap-ratio with the singular density of states of the form

$N(\varepsilon) = A|\varepsilon|^{\beta}$, have $\varepsilon = E - E_F$, and found a slow decrease of the value R from R=4 at

$\beta=-0.8$ to a low R=2.9 at $\beta=1$. Abrikosov et al.(1993), using the observed extended saddle point singularities along Γ-Y symmetry direction in a 1-2-3 high-T_c superconductor showed that the DOS diverges as the square root of energy. Using the Eliashberg theory and a model DOS of the form , Zeyhar(1995) showed that large enhancements of T_c and strong reductions of the isotope exponent cannot be explained.

Gap-to-T_c Ratio

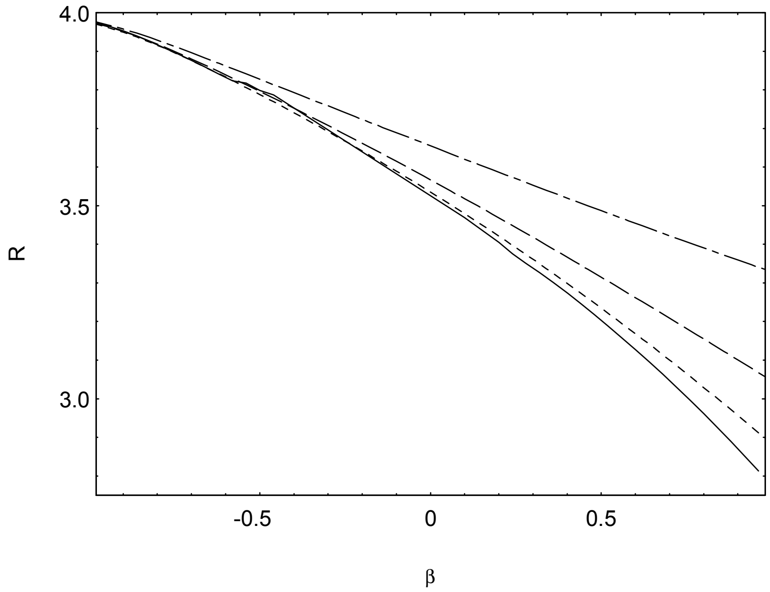
Udomsamuthirun et al.(1996) used the singularity density of states of the form, $N(\varepsilon) = A|\varepsilon|^{\beta}$ where $\varepsilon = E - E_F$. They obtained the exact formula for R :

$$R = 4\left[\frac{\int_0^{\omega_D/2T_c} dx\, x^{-1+\beta} \tanh x}{\int_0^{2\omega_D/RT_c} dx\, x^{-1+\beta} (1+1/x^2)^{-1/2}}\right]^{1/\beta} \qquad (4.20)$$

for $\beta<0$, and $\beta>0$, They have

$$R = 4\left[\frac{\int_0^{\omega_D/2T_c} dx\, x^{-1+\beta} (1-\tanh x)}{\int_0^{2\omega_D/RT_c} dx\, x^{-1+\beta} (1-(1+1/x^2)^{-1/2})}\right]^{1/\beta} \qquad (4.21)$$

A numerical calculation of R based on Eqs.(4.20) and (4.21) is shown in Figure(4.3) as a function of β for different value of ω_D/T_c .



Figure(4.3) Plot of $R=2\Delta_0/T_c$ for different choices of ω_D/T_c as a function of the exponent β .$\omega_D/T_c \rightarrow \infty$ (—) , $\omega_D/T_c \rightarrow 754/40$ (-----), $\omega_D/T_c \rightarrow 754/90$ (— — —), and $\omega_D/T_c \rightarrow 754/90$ (——–——–) (Udomsamuthirun et al.,1996) .

At this step, we can derive Eqs.(4.20) and (4.21) for an exact solution of R and get

$$\int_0^{\omega_D/2T_c} dx\, x^{\beta-1} \tanh x = \sum_{n=0}^{\infty} \left(\pi(n+\frac{1}{2})\right)^{\beta-1} B_x\left(\frac{\beta+1}{2}, \frac{1-\beta}{2}\right); x = \frac{\omega_D^2}{\omega_D^2 + (2\pi T_c(n+1/2))^2}$$

$$\int_0^{2\omega_D/RT_c} dx \frac{x^\beta}{\sqrt{1+x^2}} = \frac{1}{2} B_{x_1}\left(\frac{\beta+1}{2}, \frac{\beta}{2}\right)$$

For $\beta<0$, we obtain

$$R = 4\left[\frac{\sum_{n=0}^{\infty} \left(\pi(n+\frac{1}{2})\right)^{\beta-1} B_x\left(\frac{\beta+1}{2}, \frac{1-\beta}{2}\right)}{\frac{1}{2} B_{x_1}\left(\frac{\beta+1}{2}, \frac{\beta}{2}\right)}\right]^{1/\beta} \tag{4.22}$$

and for $\beta>0$, we obtain

$$R = 4\left[\frac{\frac{1}{\beta}\left(\frac{\omega_D}{2T_c}\right)^\beta - \sum_{n=0}^{\infty} \left(\pi(n+\frac{1}{2})\right)^{\beta-1} B_x\left(\frac{\beta+1}{2}, \frac{1-\beta}{2}\right)}{\frac{1}{\beta}\left(\frac{\omega_D}{2T_c}\right)^\beta - \frac{1}{2} B_{x_1}\left(\frac{\beta+1}{2}, \frac{\beta}{2}\right)}\right]^{1/\beta} \tag{4.23}$$

Isotope Effect

Consider density of states of form

$$N(E) = N_0 \left| \frac{E - E_F}{E_F} \right|^{\beta} \tag{4.24}$$

At $T=T_c$, substitution Eq.(4.24) into Eq.(4.1), $x=(E-E_F)/2T_c$ and $\Delta(T_c)=0$,

$$\frac{E_F^{\beta}}{N_0 V} = (2T_c)^{\beta} \int_0^{\omega_D/2T_c} dx\, x^{\beta-1} \tanh x \tag{4.25}$$

Differentiation Eq.(4.25) with respect to ω_D all the way, we find

$$\frac{\partial T_c}{\partial \omega_D} = \frac{\omega_D^{\beta-1} \tanh(\frac{\omega_D}{2T_c})}{\frac{\omega_D^{\beta}}{T_c} \tanh(\frac{\omega_D}{2T_c}) - \beta 2^{\beta} T_c^{\beta-1} \int_0^{\omega_D/2T_c} dx\, x^{\beta-1} \tanh x} \tag{4.26}$$

We have $\int_0^{\omega_D/2T_c} dx\, x^{\beta-1} \tanh x = 2\sum_{n=0}^{\infty} \int_0^{\omega_D/2T_c} dx \frac{x^{\beta}}{x^2 + (\pi(n+\frac{1}{2}))^2}$

$$= 2\sum_{n=0}^{\infty} \int_0^{\theta_m} d\theta [\pi(n+\frac{1}{2})]^{\beta-1} \tan^{\beta}\theta$$

$$= \sum_{n=0}^{\infty} [\pi(n+\frac{1}{2})]^{\beta-1} B_x(\frac{\beta+1}{2}, \frac{1-\beta}{2})$$

where $\theta_m = \tan^{-1}(\frac{\omega_D}{2\pi T_c (n+\frac{1}{2})})$, $x = \frac{\omega_D^2}{\omega_D^2 + (2\pi T_c (n+\frac{1}{2}))^2}$, and

$$B_y(p,q) = \int_0^y dt\, t^{p-1}(1-t)^{q-1} = 2 \int_0^{\arcsin\sqrt{y}} \sin^{2p-1}\theta \cos^{2q-1}\theta d\theta$$

B_y is the incomplete beta function .

We find

$$\alpha = \frac{1}{2} \frac{\tanh(\frac{\omega_D}{2T_c})}{[\tanh(\frac{\omega_D}{2T_c}) - \beta(\frac{2T_c}{\omega_D})^{\beta} \sum_{n=0}^{\infty} (\pi(n+\frac{1}{2}))^{\beta-1} B_x(\frac{\beta+1}{2}, \frac{1-\beta}{2})]} \tag{4.27}$$

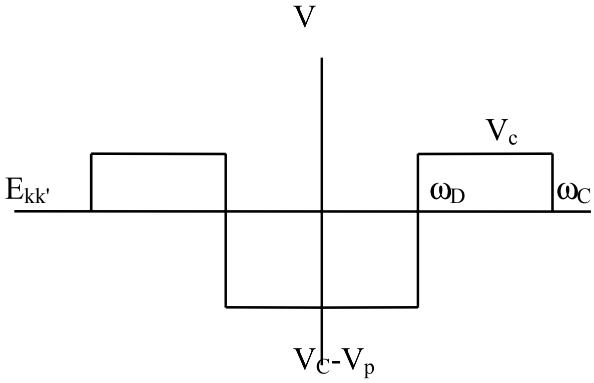
The Effect of Coulomb Repulsion on T_c

In this section we will show the development of the Cooper model potential which qualitatively accounts for the effects of Coulomb repulsion (Ketterson and Song, 1999). We have the BCS gap equation as

$$\Delta(E_{k'}) = N_0 \int V(E_{kk'})\Delta(E_k)\frac{\tanh(\frac{E_k}{2T_c})}{E_k} dE_k \tag{4.28}$$

We introduce the Bogoliubov model (Bogoliubov et al., 1958) potential shown in Figure(4.4), which may write as

$$V(E_{kk'}) = \begin{cases} -V_p + V_c & \text{for } -\omega_D < E_{kk'} < \omega_D \\ +V_c & \text{for } \omega_D < |E_{kk'}| < \omega_c \end{cases} \tag{4.29}$$



Figure(4.4) Schematic diagram of the Bogoliubov model potential.

The differs from the Cooper potential (which contains only the attractive component -Vp) by the addition of a constant repulsive potential, $+V_c$, in the interval $\omega_D < E_{kk'} < \omega_c$ where ω_c is a Coulomb cut-off frequency.

The function $\Delta(E_k)$ will be described in terms of two values Δ_1 and Δ_2 as follows :

$$\Delta(E_k) = \begin{cases} \Delta_1 & \text{for } -\omega_D < E_k < \omega_D \\ \Delta_2 & \text{for } \omega_D < |E_k| < \omega_c \end{cases} \tag{4.30}$$

Consider when $E_k < \omega_D$, we can get

$$\Delta_1 = \Delta_1 \int_0^{\omega_D} d\varepsilon N_0(-V_p + V_c)\frac{\tanh(\varepsilon / 2T_c)}{\varepsilon} + \Delta_2 \int_{\omega_c}^{\omega_D} d\varepsilon N_0 V_c \frac{\tanh(\varepsilon / 2T_c)}{\varepsilon} \tag{4.31}$$

and when $E_k > \omega_D$, we get

$$\Delta_2 = \Delta_1 \int_0^{\omega_D} d\varepsilon N_0 V_c \frac{\tanh(\varepsilon/2T_c)}{\varepsilon} + \Delta_2 \int_{\omega_c}^{\omega_D} d\varepsilon N_0 V_c \frac{\tanh(\varepsilon/2T_c)}{\varepsilon} \tag{4.32}$$

The above equations can be write into 2x2 matrix as :

$$\begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix} = \begin{pmatrix} I_{11} & I_{12} \\ I_{21} & I_{22} \end{pmatrix} \begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix} \tag{4.33}$$

here

$$\begin{aligned} I_{11} &= N_0(-V_p + V_c) \int_0^{\omega_D} d\varepsilon \frac{\tanh(\varepsilon/2T_c)}{\varepsilon} \\ &= N_0(-V_p + V_c) \ln(\frac{1.13\omega_D}{T_c}) \\ I_{12} &= N_0 V_c \int_{\omega_c}^{\omega_D} d\varepsilon \frac{\tanh(\varepsilon/2T_c)}{\varepsilon} \\ &= N_0 V_c \ln(\frac{\omega_c}{\omega_D}) = I_{21} \end{aligned}$$

and $$I_{22} = N_0 V_c \ln(\frac{1.13\omega_D}{T_c})$$

Introducing the parameter $\lambda = N_0 V_p$ and $\mu = N_0 V_c$ the critical temperature can be obtained from the solution of

$$\begin{vmatrix} (\lambda-\mu)\ln(\frac{1.13\omega_D}{T_c}) - 1 & -\mu\ln(\frac{\omega_c}{\omega_D}) \\ -\mu\ln(\frac{1.13\omega_D}{T_c}) & -\mu\ln(\frac{\omega_c}{\omega_D}) \end{vmatrix} = 0 \tag{4.34}$$

Setting the determinant to zero yields the condition

$$1 + \mu\ln(\frac{\omega_c}{\omega_D}) - \lambda\ln(\frac{1.13\omega_D}{T_c})(1 + \mu\ln(\frac{\omega_c}{\omega_D})) + \mu\ln(\frac{1.13\omega_D}{T_c}) = 0$$

Introducing a quantity $\mu^* = \dfrac{\mu}{1+\mu\ln(\omega_c/\omega_D)}$, we get T_c 's equation within the Coulomb repulsion as

$$T_c = 1.13\omega_D \exp\{-[\frac{1}{\lambda-\mu^*}]\} \tag{4.35}$$

The isotope effect can be obtained by differential Eq.(4.35) with respect to ω_D . We find that

$$\frac{\partial T_c}{\partial \omega_D} = \frac{T_c}{\omega_D}[1-\frac{\mu^2}{1+\mu\ln(\omega_c/\omega_D)}] \tag{4.36}$$

then the isotope exponent is

$$\alpha = \frac{1}{2}[1-\frac{\mu^2}{1+\mu\ln(\omega_c/\omega_D)}] \tag{4.37}$$

For the present of Coulomb repulsion, the isotope exponent is decrease from the pure electron-phonon interaction, α=1/2, that agree with experiment for the conventional superconductor .

The Short-range Pairing Interaction

Yoksan (1991) purpose the influence of logarithmic singularity density of states as well as the short range interaction on the isotope effect exponent.

This kind of density of state occurred when we consider the Hubbard model on a two-dimensional square lattice that

$$H = -\sum_{ij\sigma} t\, c^+_{i\sigma} c_{j\sigma} + U\sum_i n_{i\uparrow} n_{i\downarrow} \tag{4.38}$$

here t denotes the transfer integral, and U the renormalized on site Coulomb interaction, the number operator $n_{i\sigma} = c^+_{i\sigma} c_{i\sigma}$. In case of the nearest neighbour hopping, the band energy is $E(k) = -2t(\cos k_x + \cos k_y)$. This gives rise to the density of states in the form

$$N(E) = \begin{cases} \frac{1}{2\pi^2 t} K[1-(\frac{E}{4t})^2]^{1/2} & |E| < 4t \\ 0 & |E| > 4t \end{cases} \quad (4.39)$$

when K is the complete elliptic integral of the first kind, and N(E) is non-zero only when $0 < E < 4t$, for $E \approx 0$, N(E) takes the form

$$N(E) = -\frac{1}{2\pi^2 t} \ln\left|\frac{E}{16t}\right| \quad (4.40)$$

Here $N(\omega_D)$ is analogous to the density of states at the Fermi level of the BCS theory.

He assumed the short range pairing interaction of form

$$V_{kk'} = \begin{cases} -V_1 - V_2 & ,\text{for} \quad 0 < E < \omega_D \\ -V_2 & ,\text{for} \quad \omega_D < E < 4t \end{cases} \quad (4.41)$$

is independent of the phonon frequency. Here V_1 is the phonon-mediated interaction and V_2 is the extra interaction which may be of nonelectron-phonon origin. E is the electron energy measured from the Fermi energy, ω_D is the Debye cut-off energy and 4t is the energy cut-off for V_2 .

Considering in the BCS scenario, we can use the BSC gap's equation as

$$\Delta(k) = \frac{1}{2}\sum_q \frac{V(k-q)\Delta(q)}{\sqrt{E^2+\Delta^2(q)}} \tanh(\frac{\sqrt{E^2+\Delta^2(q)}}{2T}) \quad (4.42)$$

Based on equation (4.41) has the following form

$$\Delta(k,T) = \begin{cases} \Delta_0(T)\Delta_1 & ,\text{if } E < \omega_D \\ \Delta_0(T)\Delta_2 & ,\text{if } E > \omega_D \end{cases} \quad (4.43)$$

Here Δ_1 and Δ_2 are temperature-independent constants. Upon substitution equation (4.43) into (4.42), we obtain the following equations

$$\Delta_1[1-(V_1+V_2)\Sigma_1(T)] = \Delta_2 V_2 \Sigma_2(T)$$
$$\Delta_1 V_2 \Sigma_1(T) = \Delta_2[1-V_2\Sigma_2(T)] \qquad (4.44)$$

when

$$\Sigma_1(T) = \int_0^{\omega_D} dE \frac{N(E)}{\sqrt{E^2+\Delta_0^2\Delta_1^2}} \tanh\left(\frac{\sqrt{E^2+\Delta_0^2\Delta_1^2}}{2T}\right)$$
$$\Sigma_2(T) = \int_{\omega_D}^{4t} dE \frac{N(E)}{\sqrt{E^2+\Delta_0^2\Delta_2^2}} \tanh\left(\frac{\sqrt{E^2+\Delta_0^2\Delta_2^2}}{2T}\right) \qquad (4.45)$$

We obtain Eq.(4.45) by replacing the summation over q by the energy integral.

At $T=T_c$, $\Delta_0(T_c)=0$, with the aid of the expression for N(E) we can see that integrals in Eq.(4.45) are dominant around E=0, so we approximated Eq.(4.45) as

$$\Sigma_1(T_c) = -\frac{1}{2\pi^2 t} F\left(\frac{\omega_D}{2T_c}\right)$$

and

$$\Sigma_2(T_c) = -\frac{1}{2\pi^2 t}\left\{F\left(\frac{4t}{2T_c}\right) - F\left(\frac{\omega_D}{2T_c}\right)\right\}$$

which the function F is defined by (Labbe and Bok, 1987)

$$F\left(\frac{y}{2T_c}\right) = \int_0^{y/16t} dx \frac{\ln x}{x} \tanh\left(\frac{8tx}{T_c}\right)$$
$$= -\frac{1}{2}\ln^2\left(\frac{T_c}{8t}\right) + 0.819\,\ln\left(\frac{T_c}{8t}\right) + \frac{1}{2}\ln^2\left(\frac{\omega_D}{16t}\right) - 1\ .$$

When Eq.(4.44) are compatible we arrive at the following condition

$$1+\lambda F\left(\frac{\omega_D}{2T_c}\right) + \sigma F\left(\frac{4t}{2T_c}\right) + \lambda\sigma F\left(\frac{\omega_D}{2T_c}\right)\left[F\left(\frac{4t}{2T_c}\right) - F\left(\frac{\omega_D}{2T_c}\right)\right] = 0 \qquad (4.46)$$

here we have introduced the variables $\lambda = \frac{V_1}{2\pi^2 t}$ and $\sigma = \frac{V_2}{2\pi^2 t}$.

Putting F in Eq.(4.46) and rearranging, one arrives at the equation for T_c .

$$T_c = 1.13\omega_D \exp\{\frac{\frac{1}{\lambda+\sigma^*} - 0.6646}{\ln(\omega_D / 16t)}\} \tag{4.47}$$

where

$$\sigma^* = \frac{\sigma}{1 - \frac{\sigma}{2}\ln(\frac{4t}{\omega_D})\ln(\frac{64t}{\omega_D})}$$

The isotope effect exponent can be derived from Eq.(4.47) as

$$\alpha = \frac{d\ln T_c}{d\ln M}$$

$$= \frac{1}{2}\{1 - [1 - \lambda(0.6646 + \ln(\frac{\omega_D}{16t})\ln(\frac{T_c}{1.134\omega_D}))]^2 - \frac{\ln(T_c / 1.134\omega_D)}{\ln(\omega_D / 16t)}\} \tag{4.48}$$

In the limit of low T_c , it is straight forward to show that Eq.(4.48) can be estimated as

$$\alpha = \frac{1}{2}\{1 - [1 - \lambda\ln(\frac{\omega_D}{16t})\ln(\frac{T_c}{1.134\omega_D})]\}$$

here the quantity $\left|\frac{V_1}{2\pi^2 t}\ln(\frac{\omega_D}{16t})\right|$ in our model is equivalent to N_0V_1 in Eq.(12) of Daemen and Overhauser (1990).

In conclusion, he found that the singularity contributes to the conspicuous enhancement of T_c. He also found that the behavior of the exponent α depends sensitively on the relative magnitudes of the two interactions. The isotope effect decreases as the ratio V_1/V_2 decreases and increases as the ratio V_1/V_2 increases. The zero isotope effect can be achieved both for high and low T_c materials.

CHAPTER V

THE ISOTOPE EFFECT IN HIGH-T_c SUPERCONDUCTOR

It has been observed that the critical temperature of a superconductor varies with isotope mass (Justi,1941). In mercury, T_c varies from 4.185 K to 4.146 K as the average isotope mass M varies from 199.5 to 203.4 atomic mass units (Kittel,1991) . The transition temperature is found to change smoothly when we mix different isotopes of the same element. The experimental results within each series of isotopes may be fitted by a relation of the form $M^{\alpha}T_c$ = constant (α called the isotope exponent).

The BCS theory (Bardeen, Cooper,and Schrieffer,1957) found that $T_c \alpha M^{-1/2}$, M is atomic mass, or α=1/2 .

This relationship is obeyed very well by wide range of conventional superconductors. The results obtained on measuring the isotope exponent are summarized for several conventional superconductors in Table(1.2).

Experimental Results

Isotope effects have been measured in the high-T_c superconductors, most commonly by varying the oxygen isotope as replacing ^{16}O with ^{18}O because it is thought that O-atom vibrations(the highest-frequency phonons) might be responsible for the major part of the electron-phonon interaction. The result is that the isotope effect is strongly dependent on the hole doping. Some optimally doped samples show a very small isotope exponent of the order of 0.05 or even smaller (Batlogg et al., 1987) and some samples show a higher value than 0.5 in contrast to the conventional value of 0.5 or less which one expects for a conventional phonon induced pairing interaction (Franck,1994).

Reports on the isotope exponent, α, of a high-T_c superconductor is shown in Table below, here x is doping concentration.

x(%)	T_c(K)	α
0	92.3	0.025
10	91.9	0.039
20	77.3	0.140
30	73	0.213
30	60	0.269
40	49.3	0.324
50	38.3	0.380

Table(5.1) Dependence of α on T_c in Y Ba_{2-x} $La_xCu_3O_{7-\delta}$ system (Bornemann and Morris, 1991).

Bornemann and Morris (1991) reported the dependence of the oxygen isotope shift on the critical temperature in the system Y Ba_{2-x} $La_xCu_3O_{7-\delta}$ with $0 \le x \le 0.5$. They found a significant oxygen isotope shift at low temperatures (α=0.38 at T_c=38.3 K) which decreases gradually with increasing T_c and finally falls rapidly above 73 K to α=0.025 for T_c =92.3 K. Their results suggest a dominant role for conventional electron-phonon coupling in the high-T_c cuprate superconductors .

x(%)	T_c(K)	α
20	75.6	0.09
30	60.4	0.15
40	46.2	0.27
50	30.6	0.45

Table(5.2) Dependence of α on T_c in (Y_{1-x} Pr_x)$Ba_2Cu_3O_{7-\delta}$ system (Franck, Jung, and et.al., 1991).

Franck, Jung and et.al. (1991) studied the oxygen isotope effect in the system $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$. They found that the oxygen isotope exponent α increases with increasing x and therefore decreasing critical temperature T_c . For the highest Pr concentrations α tends toward α=0.5 . The value of the isotope exponent depends on the concentration of mobile holes. The lower this concentration is , the larger becomes the isotope exponent. They concluded that ,in the $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$ system, lattice vibrations dominated by oxygen apparently play an important role in the behavior of high-T_c superconductors.

x(%)	T_c(K)	α
20	74.9	0.09
30	59.6	0.24
40	45.8	0.32
50	27.7	0.79

Table(5.3) Dependence of α on T_c in $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$ system (Soerensen and Gygax, 1995).

z(%)	T_c(K)	α
20	67.5	0.04
25	63.0	0.04
40	55.4	0.07
50	38.5	0.02
60	29.4	0.09
70	19.1	0.12
75	12.7	0.13

Table(5.4) Dependence of α on T_c in $YBa_2(Cu_{1-z}Zn_z)_3O_{7-\delta}$ system (Soerensen and Gygax, 1995) where z is doping concentration.

x(%)	y(%)	$T_c(K)$	α
20	0	67.5	0.14
20	5	63.0	0.08
20	10	55.4	0.09
20	15	38.5	0.05
20	20	29.4	0.08
20	25	19.1	0.06

Table(5.5) Dependence of α on T_c in $(Y_{1-x-y}Pr_xCa_y)Ba_2Cu_3O_{7-\delta}$ system (Soerensen and Gygax, 1995) where x and y are doping concentration.

Soerensen and Gygax (1995) measured the oxygen isotope exponent in $YBa_2Cu_3O_7$ substituted with Pr, Ca, and Zn and analyzed it in detail. They found that for the Pr and Pr : Ca substitutions there is a correlation between the isotope shift and the width of the transition. This suggests that the upturn in the isotope exponent for Pr substitutions could be due, at least partially, to a sample quality problem. They also point out that a linear extrapolation to 100% ^{18}O substitution results in an overestimate of the isotope exponent.

x(%)	$T_c(K)$	α
7.5	24.0	0.30
9.0	29.3	0.53
10.0	29.2	0.62
15.0	29.1	0.21
17.5	24.6	0.11

Table(5.6) Dependence of α on T_c in $La_{2-x}Ba_xCuO_4$ system (Crawford et al.,1990) .

x(%)	T_c(K)	α
12	29.4	0.78
13	34.4	0.57
14	36.9	0.15

Table(5.7) Dependence of α on T_c in $La_{2-x} Sr_xCuO_4$ system (Crawford et al., 1990) .

Crawford et al. (1990) studied the oxygen isotope effect on in $La_{2-x} Ba_xCuO_4$ and $La_{2-x} Sr_xCuO_4$ system. They found the maximum α values (α >0.5) for x near 12 %.

Theoretical Survey

The explanation for the isotope effect in high-T_c cuprate superconductors remains obscure though there are many possible explanations for its unusual doping dependence (Franck, 1994). Experimentally it is found that optimally doped samples show a very small isotope exponent α of the order 0.05 or even smaller (Batlogg et al., 1987) . This unusually small value in connection with the high value T_c leads to early suggestion that the pairing interaction in high-T_c cuprates might be predominantly electronic in origin with a possible small phononic contribution (Marsiglio et al., 1987) . This scenario is difficult to reconcile with the fact that some isotope exponents also show unusually high values, reaching values of 0.5 or even higher in some doping superconductors (Dahm, 2000).

In recent years, researchers found the existence of a pseudogap in the normal state of underdoped high-T_c cuprate superconductors for gaplike structure in the normal state at temperature T*, $T^* > T_c$. And pseudogap develops into superconducting gap below T_c .

To explain the unusual isotope effect of cuprate both smaller, almost absence, and higher than the conventional value 0.5, many models have been proposed such as the van Hove singularity (Labbe and Bok, 1987; Tsuei et al., 1990; Radtke and

Norman, 1994), anharmonic phonon (Schuttler and Pao, 1995; Pietronero and Strassler, 1992), and pairing breaking effect (Carbotte et al., 1991) . Recently, Dahm (Dahm, 2000) studied the influence of the pseudogap on the isotope exponent having an electronic pairing interaction with a subdominant electron-phonon interaction. In the weak-coupling limit, he found that the introduction of a pseudogap leads to strong increase of isotope exponent above its values in the absence of a pseudogap. He performs his study numerically.

The purpose of this research is to explain the unusual isotope effect of cuprates both smaller and higher than 0.5 by considering the influence of the pseudogap and subdominant electron-phonon interaction in the weak-coupling limit. We will derive exact formula of the isotope exponent for the superconductor having a constant and power law density of states.

Within the simple model of Loram et al. (1994) superconductivity gap and normal-state pseudogaps are assumed to arise from independent and competing correlations and hence the superconducting gap can be written as

$$\Delta^2(T) = \Delta'^2(T) + E_g^2 \tag{5.1}$$

where $\Delta'(k)$ is the superconducting order parameter and E_g is the normal-state pseudogap. Therefore at $T=T_c$, $\Delta(T_c)=E_g$ and the linearized gap equation in the weak-coupling limit for an anisotropic pairing interaction V(k,k') read

$$\Delta'(k) = \sum_{k'} V(k,k') \frac{\tanh(\sqrt{\varepsilon_{k'}{}^2 + E_g^2} / 2T_c)}{2\sqrt{\varepsilon_{k'}{}^2 + E_g^2}} \Delta'(k') \quad . \tag{5.2}$$

Here ε_k is the band dispersion and V(k,k') is the pairing interaction .

We introduce the short-range interaction by following closely the work of Dahm (2000) . We assume that the pairing interaction consists of two parts : a phononic part $V_p(k,k')$ and an electron part $V_e(k,k')$, such that the pairing interaction

$$V(k,k') = V_p(k,k') + V_e(k,k') \tag{5.3}$$

The dominant contribution should be V_e. We have

$$V_{e,p}(k,k') = \begin{cases} V_{e0,p0}\Psi_\eta(k)\Psi_\eta(k') & \text{if} |\varepsilon_k|,|\varepsilon_{k'}| \le \omega_{e,p} \\ 0 & \text{else} \end{cases} \quad (5.4)$$

here ω_e and ω_p is the characteristic energy cutoff of the electronic part and phononic part respectively. ω_e is assumed to be independent of the isotopic mass and ω_p varies with isotopic mass M like $1/\sqrt{M}$ as in the harmonic approximation. $\Psi_\eta(k)$ is the basis function for the pairing symmetry considered and

$$\Psi_\eta(k) = 1 \quad \text{for s-wave pairing,}$$

$$= \cos 2\theta_k \quad \text{for } d_{x^2-y^2} \text{ wave pairing,} \quad (5.5)$$

where $\theta = \tan^{-1}(\frac{k_y}{k_x})$ is the angular direction of the momentum k in the ab plane.

In our basis function, we have s-wave pairing that is always found in conventional superconductors and $d_{x^2-y^2}$ wave pairing that is found in cuprates .

For such an interaction the superconducting order parameter can be separated into two parts : $\Delta(k) = \Delta_e(k) + \Delta_p(k)$ with

$$\Delta_{e,p}(k) = \begin{cases} \Delta_{e0,p0}\Psi_\eta(k) & \text{if} |\varepsilon_k| \le \omega_{e,p} \\ 0 & \text{else} \end{cases}. \quad (5.6)$$

Because it is widely accepted that the pseudogap in cuprate occurs below a certain temperature T^*, which is much higher than T_c (Timusk and Statt,1999) so we can assume that $T^* > \omega_p > \omega_e$. We also assume that $\Delta(k)$ and $E_g(k)$ have the same symmetry (Ding et al., 1996; Williams et al., 1997; Loeser et al., 1996) , so we choose $E_g(k)$ to be

$$E_g(k) = \begin{cases} E_{g0} & \text{for s-wave} \\ E_{g_0}\cos(2\theta_k) & \text{for d-wave} \end{cases} \quad (5.7)$$

where E_{go} is constant.

With this ansatz Eq.(5.2) becomes a 2x2 matrix equation for the two order-parameter components Δ_{e0} and Δ_{p0} by using the condition $\omega_p > \omega_e$, we arrive at the following equation,

$$\begin{pmatrix} \Delta_{e0} \\ \Delta_{p0} \end{pmatrix} = \begin{pmatrix} V_{e0}L(\omega_e, T_c) & V_{e0}L(\omega_e, T_c) \\ V_{p0}L(\omega_e, T_c) & V_{p0}L(\omega_p, T_c) \end{pmatrix} \begin{pmatrix} \Delta_{e0} \\ \Delta_{p0} \end{pmatrix} \tag{5.8}$$

where

$$L(\omega, T_c) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \psi_\eta^2(\theta) \int_0^{\omega} d\varepsilon \frac{N(\varepsilon)}{\sqrt{\varepsilon^2 + E_g^2}} \tanh\left(\frac{\sqrt{\varepsilon^2 + E_g^2}}{2T_c}\right) \quad . \tag{5.9}$$

The solution of Eq.(5.8) is

$$\lambda(\omega_e, \omega_p, T_c) = \frac{V_{e0}L_e + V_{p0}L_p}{2} + \frac{1}{2}\sqrt{(V_{e0}L_e - V_{p0}L_p)^2 + 4V_{e0}V_{p0}{L_e}^2} \tag{5.10}$$

where $L_e = L(\omega_e, T_c)$ and $L_p = L(\omega_p, T_c)$.

T_c is determined from the implicit equation

$$\lambda(\omega_e, \omega_p, T_c) = 1 \tag{5.11}$$

From Eqs.(5.10) and (5.11), the isotope exponent α can be calculated :

$$\alpha = \frac{1}{2}\frac{d}{d}\frac{\ln T_c}{\ln \omega_p} = -\frac{1}{2}\frac{\omega_p}{T_c} \frac{\frac{\partial \lambda}{\partial L_p}\frac{\partial L_p}{\partial \omega_p}}{\frac{\partial \lambda}{\partial L_p}\frac{\partial L_p}{\partial T_c} + \frac{\partial \lambda}{\partial L_e}\frac{\partial L_e}{\partial T_c}}$$

$$= \frac{-\frac{1}{2}\frac{\omega_p}{T_c}\frac{\partial L_p}{\partial \omega_p}}{\frac{\partial L_p}{\partial T_c} + \frac{V_{e0}}{V_{p0}}\left(\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}\right)\frac{\partial L_e}{\partial T_c}} \tag{5.12}$$

Isotope Exponent for a Constant DOS

For a superconductor with the constant density of states, $N(E) = N_0$ through out the Fermi energy. It is a basic DOS consideration that was firstly considered by the BCS theory. If we look closely at the calculation in detail, we will consider many cases such as s-wave without a pseudogap, s-wave with a pseudogap, d-wave without a pseudogap, and d-wave with a pseudogap.

S-Wave without a Pseudogap

Inserting a constant DOS and the condition for s-wave without pseudogap in Eq.(5.9), we get

$$L(\omega, T_c) = \int_0^{\omega} d\varepsilon \frac{N_0}{\varepsilon} \tanh(\frac{\varepsilon}{2T_c}) \tag{5.13}$$

$$= \frac{4N_0}{\pi} \sum_{n=0}^{\infty} \frac{1}{2n+1} \tan^{-1}(\frac{\omega}{2\pi T_c (n+1/2)})$$

This equation is the BCS's gap equation .

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial \omega}$ and $\frac{\partial L}{\partial T_c}$. We obtain

$$\frac{\partial L(\omega, T_c)}{\partial \omega} = \frac{N_0}{\omega} \tanh(\frac{\omega}{2T_c}) \tag{5.14}$$

and

$$\frac{\partial L(\omega, T_c)}{\partial T_c} = -\frac{N_0}{T_c} \tanh(\frac{\omega}{2T_c}) \tag{5.15}$$

Substituting Eq.(5.14) and Eq.(5.15) into Eq.(5.12), we find the s-wave isotope exponent without a pseudogap as

$$\alpha_{s0} = \frac{\frac{1}{2}\tanh(\frac{\omega_p}{2T_c})}{\tanh(\frac{\omega_p}{2T_c}) + \frac{V_{e0}}{V_{p0}}[\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}]\tanh(\frac{\omega_e}{2T_c})} \tag{5.16}$$

where $L(\omega,T_c)$ is defined by Eq.(5.13) and $L_p=L(\omega_p,T_c)$, and $L_e=L(\omega_e,T_c)$.

For a purely electronic interaction, $V_{p0}=0$, Eq.(5.16) gives $\alpha=0$ and for a purely phononic interaction, $V_{e0}=0$, it gives $\alpha= 1/2$ that is the BCS' result, it also agrees with the Dahm 's (2000) result.

S-Wave with a Pseudogap

In this case, we assume that $\Delta^2(T) = \Delta'^2(T) + E_{g0}^2$ and for T=T$_c$,superconducting gap is equal to zero then $\Delta(T_c) = E_{g0}$. Inserting a constant DOS and the condition for a pseudogap in Eq.(5.9), we get

$$L(\omega, T_c) = \int_0^{\omega} d\varepsilon \frac{N_0}{\sqrt{\varepsilon^2 + E_{g0}^2}} \tanh\left(\frac{\sqrt{\varepsilon^2 + E_{g0}^2}}{2T_c}\right) \tag{5.17}$$

$$= 4N_0 T_c \sum_{n=0}^{\infty} \frac{1}{\sqrt{E_{g0}^2 + a^2}} \tan^{-1}\left(\frac{\omega}{\sqrt{E_{g0}^2 + a^2}}\right)$$

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial \omega}$ and $\frac{\partial L}{\partial T_c}$. We obtain

$$\frac{\partial L(\omega_p, T_c)}{\partial \omega_p} = \frac{N_0}{\sqrt{\omega_p^2 + E_{g0}^2}} \tanh\left(\frac{\sqrt{\omega_p^2 + E_{g0}^2}}{2T_c}\right) \tag{5.18}$$

and

$$\frac{\partial L(\omega, T_c)}{\partial T_c} = \frac{L(\omega, T_c)}{T_c} - \sum_{n=0}^{\infty} 8N_0 a^2 \int_0^{\omega} d\varepsilon \frac{1}{[\varepsilon^2 + E_{g0}^2 + a^2]^2}$$

$$= \frac{L(\omega, T_c)}{T_c} - \sum_{n=0}^{\infty} \frac{4N_0 a^2}{E_{g0}^2 + a^2}\left[\frac{\tan^{-1}(\omega / \sqrt{E_{g0}^2 + a^2})}{\sqrt{E_{g0}^2 + a^2}} + \frac{\omega}{\omega^2 + E_{g0}^2 + a^2}\right] \tag{5.19}$$

Here we let $a = 2\pi T_c(n+1/2)$.

Since

$$\sum_{n=0}^{\infty} \frac{a^2}{(a^2 + E_{g0}^2)(a^2 + E_{g0}^2 + \omega^2)} = \frac{1}{4T_c \omega^2}\left[\sqrt{\omega^2 + E_{g0}^2} \tanh\left(\sqrt{\omega^2 + E_{g0}^2} / 2T_c\right) - E_{g0} \tanh\left(\frac{E_{g0}}{2T_c}\right)\right] \tag{5.20}$$

We find the s-wave isotope exponent with a pseudogap as

$$\alpha_s = \frac{1}{2}\frac{\frac{\omega_p}{\sqrt{\omega_p^2 + E_{go}^2}}\tanh(\frac{\sqrt{\omega_p^2 + E_{go}^2}}{2T_c})}{(f_s(\omega_p) + \frac{V_{e0}}{V_{p0}}[\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}]f_s(\omega_e))} \tag{5.21}$$

where

$$\begin{aligned} f_s(\omega) = & \frac{\sqrt{\omega^2 + E_{g0}^2}}{\omega}\tanh(\frac{\sqrt{\omega^2 + E_{g0}^2}}{2T_c}) - \frac{E_{g0}}{\omega}\tanh(\frac{E_{g0}}{2T_c}) \\ & - \sum_{n=0}^{\infty}\frac{4T_c E_{g0}^2}{(E_{g0}^2 + a^2)^{3/2}}\tan^{-1}[\frac{\omega}{\sqrt{E_{g0}^2 + a^2}}] \end{aligned} \quad . \tag{5.22}$$

This equation can be reduced to the s-wave case without a pseudogap by taking $E_{g0} = 0$.

D-Wave without a Pseudogap

For a d-wave superconductor without a pseudogap, we must include the effect of the angular direction of momentum between $\overset{\omega}{k}_x$ and $\overset{\omega}{k}_y$. Inserting a constant DOS and the condition for d-wave and a pseudogap in Eq.(5.9), we get

$$\begin{aligned} L(\omega, T_c) &= \frac{1}{2\pi}\int_0^{2\pi} d\theta \psi_\eta^2(\theta)\int_0^{\omega} d\varepsilon \frac{N_0}{\varepsilon}\tanh(\frac{\varepsilon}{2T_c}) \\ &= <\psi_\eta^2(\theta)> \int_0^{\omega} d\varepsilon \frac{N_0}{\varepsilon}\tanh(\frac{\varepsilon}{2T_c}) \end{aligned} \tag{5.23}$$

For the d-wave case, $\psi_\eta(\theta) = \cos(2\theta)$ then we get $<\psi_\eta^2(\theta)> = \frac{1}{2}$.

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial \omega}$ and $\frac{\partial L}{\partial T_c}$. We obtain

$$\frac{\partial L(\omega, T_c)}{\partial \omega} = \frac{N_0}{2\omega}\tanh(\frac{\omega}{2T_c}) \tag{5.24}$$

and

$$\frac{\partial L(\omega, T_c)}{\partial T_c} = -\frac{N_0}{2T_c}\tanh(\frac{\omega}{2T_c}) \tag{5.25}$$

Substituting Eq.(5.24) and Eq.(5.25) into Eq.(5.12), we find the relation of a d-wave isotope exponent without a pseudogap as

$$\alpha_{d0} = \frac{\frac{1}{2}\tanh(\frac{\omega_p}{2T_c})}{\tanh(\frac{\omega_p}{2T_c}) + \frac{V_{e0}}{V_{p0}}[\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}]\tanh(\frac{\omega_e}{2T_c})} \tag{5.26}$$

where

$$L(\omega, T_c) = \frac{2N_0}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}\tan^{-1}(\frac{\omega}{2\pi T_c(n+1/2)}) \tag{5.27}$$

,and $L_p = L(\omega_p, T_c)$, $L_e = L(\omega_e, T_c)$.

The d-wave isotope exponent equation without a pseudogap has the same formula as the s-wave without a pseudogap equation, but

$$L(\omega,T_c) \text{ of d-wave} = (1/2)\, L(\omega,T_c) \text{ of s-wave} \tag{5.28}$$

D-Wave with a Pseudogap

For a d-wave superconductor with pseudogap, we must include the effect of the angular direction of momentum between $\vec{k}_x$ and $\vec{k}_y$ in the pseudogap condition of the d-wave superconductor. Inserting a constant DOS and the condition of a d-wave and pseudogap in Eq.(5.9), we get

$$L(\omega, T_c) = \frac{1}{2\pi}\int_0^{2\pi} d\theta \cos^2(2\theta)\int_0^{\omega} d\varepsilon \frac{N_0}{\sqrt{\varepsilon^2 + E_{g0}^2\cos^2(2\theta)}}\tanh(\frac{\sqrt{\varepsilon^2 + E_{g0}^2\cos^2(2\theta)}}{2T_c})$$

$$= \frac{2N_0T_c}{\pi}\int_0^{\omega} d\varepsilon \int_0^{2\pi} d\theta \sum_{n=0}^{\infty}\frac{1}{E_{g0}^2 + \varepsilon^2 + a^2 + [\varepsilon^2 + a^2]\tan^2(2\theta)}$$

Since we have $\int \frac{dx}{a + b\tan^2(x)} = \frac{1}{(a-b)}[x - \sqrt{\frac{b}{a}}\tan^{-1}(\sqrt{\frac{b}{a}}\tan x)]$

then we find

$$L(\omega, T_c) = \sum_{n=0}^{\infty}\frac{4N_0T_c}{E_{g0}^2}(\omega - \int_0^{\omega} d\varepsilon \sqrt{\frac{\varepsilon^2 + a^2}{\varepsilon^2 + a^2 + E_{g0}^2}}) \tag{5.29}$$

From the relation (Prudnikov et al., 1992),

$$\int_0^x dx\sqrt{\frac{x^2 + b^2}{x^2 + a^2}} = \frac{b^2}{a}F(\phi, k) - aE(\phi, k) + x\sqrt{\frac{x^2 + a^2}{x^2 + b^2}} \text{ , a>b>0 , x>0}$$

where

$$F(\phi,k)=\int_0^{\phi}\frac{d\phi}{\sqrt{1-k^2\sin^2\phi}}$$ is the elliptic integral of the first kind

and $$E(\phi,k)=\int_0^{\phi}d\phi\sqrt{1-k^2\sin^2\phi}$$ is the elliptic integral of the second kind.

We get

$$L(\omega,T_c)=\frac{4N_0T_c}{E_{g0}^2}\sum_{n=0}^{\infty}\{\omega-[\frac{a^2}{\sqrt{E_{g0}^2+a^2}}F(\beta,q)-\sqrt{E_{g0}^2+a^2}E(\beta,q)+\omega\sqrt{\frac{\omega^2+E_{g0}^2+a^2}{\omega^2+a^2}} \tag{5.30}$$

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial\omega}$ and $\frac{\partial L}{\partial T_c}$. We obtain

$$\frac{\partial L(\omega,T_c)}{\partial\omega}=\frac{\partial Eq.(5.29)}{\partial\omega}$$

$$=\frac{4N_0T_c}{E_{g0}^2}\sum_{n=0}^{\infty}(1-\sqrt{\frac{\omega^2+a^2}{\omega^2+a^2+E_{g0}^2}}) \tag{5.31}$$

and

$$\frac{\partial L(\omega,T_c)}{\partial T_c}=\frac{\partial Eq.(5.29)}{\partial T_c}$$

$$=\frac{4N_0}{E_{g0}^2}\sum_{n=0}^{\infty}\{\int_0^{\omega}d\varepsilon[1-\sqrt{\frac{\varepsilon^2+a^2}{\varepsilon^2+a^2+E_{g0}^2}}+a^2\frac{\sqrt{\varepsilon^2+a^2}}{(\varepsilon^2+a^2+E_{g0}^2)^{3/2}}$$

$$-\frac{a^2}{\sqrt{(\varepsilon^2+a^2)(\varepsilon^2+a^2+E_{g0}^2)}}]\}$$

We have $$\int_0^{\omega}d\varepsilon\frac{1}{\sqrt{(\varepsilon^2+a^2)(\varepsilon^2+a^2+E_{g0}^2)}}=\frac{1}{\sqrt{a^2+E_{g0}^2}}F(\phi,k)$$

and

$$\int_0^{\omega}d\varepsilon\frac{\sqrt{\varepsilon^2+a^2}}{(\varepsilon^2+a^2+E_{g0}^2)^{3/2}}=\frac{1}{\sqrt{a^2+E_{g0}^2}}E(\phi,k)$$

$$-\frac{E_{g0}^2}{(a^2+E_{g0}^2)}\frac{\omega}{\sqrt{(\omega^2+a^2+E_{g0}^2)(\omega^2+a^2+E_{g0}^2)}}$$

where $\phi = \tan^{-1}(\frac{\omega}{a})$ and $k = \frac{E_{g0}}{\sqrt{a^2 + E_{g0}^2}}$.

Substituting the above equation into $\frac{\partial L}{\partial T_c}$, we get

$$\frac{\partial L(\omega, T_c)}{\partial T_c} = \frac{L(\omega, T_c)}{T_c} + \frac{4N_0}{E_{g0}^2} \sum_{n=0}^{\infty} \frac{a^2}{\sqrt{a^2 + E_{g0}^2}} \{ E(\phi, k) - F(\phi, k) - \frac{\omega E_{g0}^2}{\sqrt{(E_{g0}^2 + a^2)(E_{g0}^2 + a^2 + \omega^2)(\omega^2 + a^2)}} \} \tag{5.32}$$

In this step, we can find the exact equation of the isotope exponent of a $d_{x^2-y^2}$ wave pairing with a pseudogap as

$$\alpha_d = \frac{\omega_p \sum_{n=0}^{\infty} (\sqrt{\frac{\omega_p^2 + a^2}{\omega_p^2 + E_{g0}^2 + a^2}} - 1)}{\{f_d(\omega_p) + \frac{V_{e0}}{V_{p0}} (\frac{1 - V_{p0} L_p + 2V_{p0} L_e}{1 - V_{e0} L_e}) f_d(\omega_e)\}} \tag{5.33}$$

where

$$f_d(\omega) = \frac{L(\omega, T_c) E_{g0}^2}{N_0} + \sum_{n=0}^{\infty} \frac{2a^2}{\sqrt{E_{g0}^2 + a^2}} \{E(\beta, q) - F(\beta, q) - \frac{\omega E_{g0}^2}{\sqrt{(E_{g0}^2 + a^2)(\omega^2 + a^2)(\omega^2 + E_{g0}^2 + a^2)}}\},$$

$\beta = \tan^{-1}(\frac{\omega}{2\pi T_c (n + 1/2)})$, $q = \frac{E_{g0}}{\sqrt{E_{g0}^2 + a^2}}$ and, $F(\beta,q)$ and $E(\beta,q)$ are the elliptic integral of first and second kind respectively .

In the case $E_{g0} = 0$, Eq.(5.33) gives α_{do} of a d-wave superconductor without a pseudogap.

Isotope Exponent for a Van Hove Singularity DOS

The Van Hove singularity (VHS) in the density of states is considered to be the DOS of a cuprate superconductor. Since the origin of cuprate superconductivity is to be found in CuO_2 planes, which are weakly coupled together along perpendicular axis, their electronic structure will be quasi-two-dimensional (2D). This necessarily leads to at least one VHS coinciding with saddle point in the ε(k) surface, these saddle points being present in all 2D band structures.

Let us now use a DOS of the form

$$N(E) = N_0 \ln\left|\frac{E_F}{E - E_F}\right| \tag{5.34}$$

We will consider effect of Van Hove singularity density of state on the isotope exponent of s-wave and d-wave superconductors for both cases of with a pseudogap and without a pseudogap.

S-Wave without a Pseudogap

Inserting a VHS density of states and the condition for s-wave without a pseudogap in Eq.(5.9), we get

$$L(\omega, T_c) = N_0 \int_0^{\omega} \frac{d\varepsilon}{\varepsilon} \ln(\frac{E_F}{\varepsilon}) \tanh(\frac{\varepsilon}{2T_c}) \tag{5.35}$$

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial \omega}$ and $\frac{\partial L}{\partial T_c}$. We obtain

$$\frac{\partial L(\omega, T_c)}{\partial \omega} = \frac{N_0}{\omega} \ln(\frac{E_F}{\omega}) \tanh(\frac{\omega}{2T_c}) \tag{5.36}$$

and

$$\frac{\partial L(\omega, T_c)}{\partial T_c} = -\frac{N_0}{T_c}[\ln(\frac{E_F}{\omega}) \tanh(\frac{\omega}{2T_c}) + 2\sum_{n=0}^{\infty} \frac{1}{\pi(n+1/2)} \tan^{-1}(\frac{\omega}{2\pi T_c (n+1/2)})] \tag{5.37}$$

Substituting Eq.(5.36) and Eq.(5.37) into Eq.(5.12), we find the s-wave isotope exponent without a pseudogap as

$$\alpha_{sv0} = \frac{\frac{1}{2}\ln(\frac{E_F}{\omega_p}) \tanh(\frac{\omega_p}{2T_c})}{\{f_{sv0}(\omega_p) + \frac{V_{e0}}{V_{p0}}(\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}) f_{sv0}(\omega_e)\}} \tag{5.38}$$

where

$$f_{sv0}(\omega) = \ln(\frac{E_F}{\omega})\tanh(\frac{\omega}{2T_c}) + \sum_{n=0}^{\infty} \frac{2}{\pi(n+1/2)}\tan^{-1}(\frac{\omega}{2\pi T_c(n+1/2)}) \quad .$$

S-Wave with a Pseudogap

In this case, we have used an assumption that $\Delta(T_c) = E_{g0}$. Inserting a Van Hove singularity DOS and the condition for pseudogap in Eq.(5.9), we get

$$L(\omega, T_c) = N_0 \int_0^{\omega} d\varepsilon \frac{\ln(E_F/\varepsilon)}{\sqrt{\varepsilon^2 + E_{g0}^2}} \tanh(\frac{\sqrt{\varepsilon^2 + E_{g0}^2}}{2T_c}) \tag{5.39}$$

$$= 4N_0 T_c \sum_{n=0}^{\infty} \int_0^{\omega} d\varepsilon \ln(\frac{E_F}{\varepsilon}) \frac{1}{\varepsilon^2 + E_{g0}^2 + (2\pi T_c(n+1/2))^2}$$

We can get $\frac{\partial L}{\partial \omega}$ and $\frac{\partial L}{\partial T_c}$ as

$$\frac{\partial L(\omega, T_c)}{\partial \omega} = \frac{N_0}{\sqrt{\omega^2 + E_{g0}^2}} \ln(\frac{E_F}{\omega}) \tanh(\frac{\sqrt{\omega^2 + E_{g0}^2}}{2T_c}) \tag{5.40}$$

and

$$\frac{\partial L(\omega, T_c)}{\partial T_c} = 4N_0 \sum_{n=0}^{\infty} \int_0^{\omega} d\varepsilon \ln(\frac{E_F}{\varepsilon}) \frac{1}{\varepsilon^2 + E_{g0}^2 + (2\pi T_c(n+1/2))^2}$$

$$-8N_0 \sum_{n=0}^{\infty} \int_0^{\omega} d\varepsilon \ln(\frac{E_F}{\varepsilon}) \frac{(2\pi T_c(n+1/2))^2}{[\varepsilon^2 + E_{g0}^2 + (2\pi T_c(n+1/2))^2]^2}$$

Since we have

$$\int_0^{\omega} d\varepsilon \frac{\ln(E_F/\varepsilon)}{\varepsilon^2 + a^2 + E_{g0}^2} = \frac{1}{\sqrt{E_{g0}^2 + a^2}} \{\phi_{sv} \ln(\frac{E_F}{\sqrt{E_{g0}^2 + a^2}}) + \frac{1}{2}Cl_2(2\phi_{sv}) + \frac{1}{2}Cl_2(\pi - 2\phi_{sv})\}$$

and

$$\int_0^{\omega} d\varepsilon \frac{1}{(\varepsilon^2 + a^2 + E_{g0}^2)^2} = \frac{\omega}{2(\omega^2 + a^2 + E_{g0}^2)(a^2 + E_{g0}^2)} + \frac{\phi_{sv}}{2(a^2 + E_{g0}^2)^{3/2}}$$

and

$$\int_0^{\omega} d\varepsilon \frac{\ln\varepsilon}{(\varepsilon^2 + a^2 + E_{g0}^2)^2} = \frac{1}{2(a^2 + E_{g0}^2)}[\frac{\omega\ln\omega}{\omega^2 + a^2 + E_{g0}^2} - \frac{\phi_{sv}}{\sqrt{a^2 + E_{g0}^2}} + \int_0^{\omega} d\varepsilon \frac{\ln\varepsilon}{\varepsilon^2 + a^2 + E_{g0}^2}]$$

where $\phi_{sv} = \tan^{-1}(\frac{\omega}{\sqrt{E_{g0}^2 + a^2}})$, $Cl_2(z) = -\int_0^z dx \ln|2\sin(x/2)|$ is the Clausen integral .

Note $\int_0^x dx\ \ln(\sin x) = -x\ln 2 - \frac{1}{2}Cl_2(2x)$ and $\int_0^x dx\ \ln(\cos x) = -x\ln 2 + \frac{1}{2}Cl_2(\pi - 2x)$.

From above integrations , we find

$$\frac{\partial L(\omega, T_c)}{\partial T_c} = 4N_0 \sum_{n=0}^{\infty} \{\frac{\phi_{sv} \ln E_F}{\sqrt{E_{g0}^2 + a^2}} - \frac{a^2\omega \ln(E_F/\omega)}{(\omega^2 + E_{g0}^2 + a^2)(E_{g0}^2 + a^2)}$$
$$- \frac{\phi_{sv}}{(E_{g0}^2 + a^2)^{3/2}}[a^2 \ln(eE_F) + E_{g0}^2 \ln(\sqrt{E_{g0}^2 + a^2})]$$
$$+ \frac{E_{g0}^2}{2(E_{g0}^2 + a^2)^{3/2}}[Cl_2(2\phi_{sv}) + Cl_2(\pi - 2\phi_{sv})]\} \tag{5.41}$$

Substituting of this density of states in Eq.(5.9) yields

$$\alpha_{sv} = \frac{-\frac{1}{8}\omega_D \ln(\frac{E_F}{\omega_p}) \tanh(\frac{\sqrt{\omega_p^2 + E_{g0}^2}}{2T_c})}{T_c\sqrt{\omega_p^2 + E_{g0}^2}\,(f_{sv}(\omega_p) + (\frac{V_{e0}}{V_{p0}})(\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e})f_{sv}(\omega_e))} \tag{5.42}$$

where

$$f_{sv}(\omega) = \sum_{n=0}^{\infty} \{\frac{\phi_{sv} \ln E_F}{\sqrt{E_{g0}^2 + a^2}} - \frac{a^2\omega \ln(E_F/\omega)}{(\omega^2 + E_{g0}^2 + a^2)(E_{g0}^2 + a^2)}$$
$$- \frac{\phi_{sv}}{(E_{g0}^2 + a^2)^{3/2}}[a^2 \ln(eE_F) + E_{g0}^2 \ln(\sqrt{E_{g0}^2 + a^2})]$$
$$+ \frac{E_{g0}^2}{2(E_{g0}^2 + a^2)^{3/2}}[Cl_2(2\phi_{sv}) + Cl_2(\pi - 2\phi_{sv})]\} \tag{5.43}$$

that is the s-wave isotope exponent with a pseudogap in a Van Hove superconductor.

D-Wave without a Pseudogap

For a d-wave superconductor without a pseudogap , we must include the effect of the angular direction of momentum . Inserting a VHS density of states and the condition for d-wave in Eq.(5.9), we get

$$L(\omega, T_c) = \frac{N_0}{2\pi}\int_0^{2\pi} d\theta \psi_\eta^2(\theta)\int_0^{\omega} d\varepsilon \frac{\ln(E_F/\varepsilon)}{\varepsilon}\tanh(\frac{\varepsilon}{2T_c})$$

$$= \frac{N_0}{2}\int_0^{\omega} d\varepsilon \frac{\ln(E_F/\omega)}{\varepsilon}\tanh(\frac{\varepsilon}{2T_c}) \qquad (5.44)$$

For a d-wave case, $\psi_\eta(\theta) = \cos(2\theta)$ then $< \psi_\eta^2(\theta) >= \frac{1}{2}$.

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial \omega}$ and $\frac{\partial L}{\partial T_c}$. We obtain

$$\frac{\partial L(\omega, T_c)}{\partial \omega} = \frac{N_0}{2\omega}\ln(\frac{E_F}{\omega})\tanh(\frac{\omega}{2T_c}) \qquad (5.45)$$

and

$$\frac{\partial L(\omega, T_c)}{\partial T_c} = -\frac{N_0}{2T_c}[\ln(\frac{E_F}{\omega})\tanh(\frac{\omega}{2T_c}) + 2\sum_{n=0}^{\infty}\frac{1}{\pi(n+1/2)}\tan^{-1}(\frac{\omega}{2\pi T_c(n+1/2)})]$$

$$(5.46)$$

Substituting Eq.(5.45) and Eq.(5.46) into Eq.(5.12), we can find the d-wave isotope exponent without a pseudogap as

$$\alpha_{dv0} = \frac{\frac{1}{2}\ln(\frac{E_F}{\omega_p})\tanh(\frac{\omega_p}{2T_c})}{\{f_{dv0}(\omega_p) + \frac{V_{e0}}{V_{p0}}(\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e})f_{dv0}(\omega_e)\}} \qquad (5.47)$$

where

$$f_{dv0}(\omega) = \ln(\frac{E_F}{\omega})\tanh(\frac{\omega}{2T_c}) + \sum_{n=0}^{\infty}\frac{2}{\pi(n+1/2)}\tan^{-1}(\frac{\omega}{2\pi T_c(n+1/2)})$$

Eq.(5.47) is the same as Eq.(5.38) that is the isotope exponent of s-wave without a pseudogap, but

$L(\omega,T_c)$ of d-wave =(1/2) $L(\omega,T_c)$ of s-wave (5.48)

D-Wave with Pseudogap

For a d-wave superconductor with pseudogap, we must include the effect of the angular direction of momentum in a pseudogap and the d-wave condition. Inserting a Van Hove singularity DOS and the condition of d-wave and pseudogap in Eq.(5.9), we get

$$L(\omega, T_c) = \frac{N_0}{2\pi}\int_0^{2\pi} d\theta \cos^2(2\theta) \int_0^{\omega} d\varepsilon \frac{\ln(E_F/\varepsilon)}{\sqrt{\varepsilon^2 + E_{g0}^2\cos^2(2\theta)}} \tanh(\frac{\sqrt{\varepsilon^2 + E_{g0}^2\cos^2(2\theta)}}{2T_c})$$

(5.49)

$$= \frac{2N_0T_c}{\pi}\int_0^{\omega} d\varepsilon \int_0^{2\pi} d\theta \sum_{n=0}^{\infty} \frac{\ln(E_F/\varepsilon)}{E_{g0}^2 + \varepsilon^2 + a^2 + [\varepsilon^2 + a^2]\tan^2(2\theta)}$$

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial \omega}$ and $\frac{\partial L}{\partial T_c}$. We obtain

$$\frac{\partial L(\omega, T_c)}{\partial \omega} = \frac{N_0}{2\pi}\ln(\frac{E_F}{\omega})\sum_{n=0}^{\infty}\int_0^{2\pi} d\theta \frac{4T_c}{\omega^2 + E_{g0}^2 + a^2 + (\omega^2 + a^2)\tan^2(2\theta)}$$

that the same integration is done in the case of d-wave with a pseudogap with the constant density of states, we get

$$\frac{\partial L(\omega, T_c)}{\partial \omega} = \frac{N_0T_c}{E_{g0}^2}\ln(\frac{E_F}{\omega})\sum_{n=0}^{\infty}(1 - \sqrt{\frac{\omega^2 + a^2}{\omega^2 + a^2 + E_{g0}^2}}) \quad (5.50)$$

and

$$\frac{\partial L(\omega, T_c)}{\partial T_c} = \frac{4N_0}{E_{g0}^2}\sum_{n=0}^{\infty}\int_0^{\omega} d\varepsilon \ln(\frac{E_F}{\varepsilon})[1 - \sqrt{\frac{\varepsilon^2 + a^2}{\varepsilon^2 + a^2 + E_{g0}^2}} + \frac{a^2\sqrt{\varepsilon^2 + a^2}}{(\varepsilon^2 + a^2 + E_{g0}^2)^{3/2}} - \frac{a^2}{\sqrt{(\varepsilon^2 + a^2)(\varepsilon^2 + a^2 + E_{g0}^2)}}]$$

$$= \frac{4N_0}{E_{g0}^2}\sum_{n=0}^{\infty}\int_0^{\omega} d\varepsilon \ln(\frac{E_F}{\varepsilon})[1 - \sqrt{\frac{\varepsilon^2 + a^2}{\varepsilon^2 + a^2 + E_{g0}^2}} - \frac{a^2E_{g0}^2}{\sqrt{\varepsilon^2 + a^2}(\varepsilon^2 + a^2 + E_{g0}^2)^{3/2}}]$$

(5.51)

The result of integration in Eq.(5.51) is very complicated so it is better to leave it in the integration form.

Substitution of Eq.(5.50) and Eq.(5.51) into Eq.(5.12), we can find the d-wave isotope exponent with a pseudogap as

$$\alpha_{dv} = \frac{-\frac{1}{8}\ln(\frac{E_F}{\omega})\sum_{n=0}^{\infty}(1 - \sqrt{\frac{\omega^2 + a^2}{\omega^2 + a^2 + E_{g0}^2}})}{\{f_{dv}(\omega_p) + \frac{V_{e0}}{V_{p0}}[\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}]\, f_{dv}(\omega_e)\}} \quad (5.52)$$

where

$$f_{dv}(\omega) = \frac{4N_0}{E_{g0}^2}\sum_{n=0}^{\infty}\int_0^{\omega} d\varepsilon \ln(\frac{E_F}{\varepsilon})[1-\sqrt{\frac{\varepsilon^2+a^2}{\varepsilon^2+a^2+E_{g0}^2}} - \frac{a^2E_{g0}^2}{\sqrt{\varepsilon^2+a^2}(\varepsilon^2+a^2+E_{g0}^2)^{3/2}}].$$

Isotope Exponent for a Power Law Singularity DOS

Let us now use a DOS of the form(Bhardwaj and Muthu, 2000)

$$N(E) = N_0\left|\frac{E-E_F}{E_F}\right|^{\beta} \tag{5.53}$$

where N_0 includes factors which may be required to normalize N(E) and $-1< \beta <1$. This is another form of the DOS that has a singularity point .

We will consider influence of a power law singularity in the density of states on the isotope exponent of s- and d-wave superconductors, both with and without a pseudogap.

S-Wave without a Pseudogap

Inserting a power law in the singularity density of states and the condition for s-wave without a pseudogap in Eq.(5.9), we get

$$L(\omega,T_c) = N_0\int_0^{\omega}\frac{d\varepsilon}{\varepsilon}(\frac{\varepsilon}{E_F})^{\beta}\tanh(\frac{\varepsilon}{2T_c}) \tag{5.54}$$

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial \omega}$ and $\frac{\partial L}{\partial T_c}$. We obtain

$$\frac{\partial L(\omega,T_c)}{\partial \omega} = \frac{N_0}{E_F^{\beta}}\omega^{\beta-1}\tanh(\frac{\omega}{2T_c}) \tag{5.55}$$

and

$$\frac{\partial L(\omega,T_c)}{\partial T_c} = -\frac{N_0}{T_c}(\frac{\omega}{E_F})^{\beta}\tanh(\frac{\omega}{2T_c}) + \beta N_0 T_c^{\beta-1}(\frac{2}{E_F})^{\beta}\int_0^{\omega/2T_c} dx\, x^{\beta-1}\tanh x$$

We have

$$\int_0^{\omega/2T_c} dx\, x^{\beta-1}\tanh x = \sum_{n=0}^{\infty}[\pi(n+1/2)]^{\beta-1}B_{x_1}(\frac{\beta+1}{2},\frac{1-\beta}{2})$$

Here $x_1 = \frac{\omega^2}{\omega^2+a^2}$ and $B_x(p,q)$ is the incomplete beta function given by

$$B_x(p,q) = \int_0^x dt\, t^{p-1}(1-t)^{q-1}$$

$$= 2 \int_0^{\sin(\sqrt{x})} d\theta \sin^{2p-1}(\theta)\, \cos^{2q-1}(\theta) \quad , \ x<1$$

then we get

$$\frac{\partial L(\omega, T_c)}{\partial T_c} = -\frac{N_0}{T_c}\left(\frac{\omega}{E_F}\right)^{\beta} \tanh\left(\frac{\omega}{2T_c}\right) + \beta N_0 T_c^{\beta-1}\left(\frac{2}{E_F}\right)^{\beta} \sum_{n=0}^{\infty}(\pi(n+1/2))^{\beta-1} B_{x_1}\left(\frac{\beta+1}{2}, \frac{1-\beta}{2}\right) \tag{5.56}$$

Substitution of Eq.(5.55) and Eq.(5.56) into Eq.(5.12), one finds the s-wave isotope exponent without a pseudogap as

$$\alpha_{sp0} = \frac{\frac{1}{2}\omega_p^{\beta} \tanh\left(\frac{\omega_p}{2T_c}\right)}{\left\{f_{sp0}(\omega_p) + \frac{V_{e0}}{V_{p0}}\left[\frac{1 - V_{p0}L_p + 2V_{p0}L_e}{1 - V_{e0}L_e}\right] f_{sp0}(\omega_e)\right\}} \tag{5.57}$$

where $f_{sp0}(\omega) = \omega^{\beta} \tanh\left(\frac{\omega}{2T_c}\right) - 2\beta T_c \sum_{n=0}^{\infty} a^{\beta-1} B_{x_1(\omega)}\left(\frac{\beta+1}{2}, \frac{1-\beta}{2}\right)$.

If β=0 and V_{e0}=0, Eq.(5.57) is reduced to be the BCS's result .

S-Wave with a Pseudogap

In this case, we assume that $\Delta(T_c) = E_{g0}$. Inserting a power law singularity DOS and the condition for a pseudogap in Eq.(5.9), we get

$$L(\omega, T_c) = \frac{N_0}{E_F^{\beta}} \int_0^{\omega} d\varepsilon \frac{\varepsilon^{\beta}}{\sqrt{\varepsilon^2 + E_{g0}^2}} \tanh\left(\frac{\sqrt{\varepsilon^2 + E_{g0}^2}}{2T_c}\right) \tag{5.58}$$

$$= \frac{4T_c N_0}{E_F^{\beta}} \sum_{n=0}^{\infty} \int_0^{\omega} d\varepsilon \frac{\varepsilon^{\beta}}{\varepsilon^2 + E_{g0}^2 + a^2}$$

$$= \frac{2N_0 T_c}{E_F^{\beta}} \sum_{n=0}^{\infty} (E_{g0}^2 + a^2)^{\frac{\beta-1}{2}} B_x\left(\frac{\beta+1}{2}, \frac{1-\beta}{2}\right)$$

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial \omega}$ and $\frac{\partial L}{\partial T_c}$ and obtain

$$\frac{\partial L(\omega,T_c)}{\partial \omega}=\frac{N_0}{E_F^{\beta}}\frac{\omega^{\beta}}{\sqrt{\omega^2+E_{g0}^2}}\tanh(\frac{\sqrt{\omega^2+E_{g0}^2}}{2T_c}) \tag{5.59}$$

and

$$\frac{\partial L(\omega,T_c)}{\partial T_c}=\frac{4N_0}{E_F^{\beta}}\sum_{n=0}^{\infty}\{\int_0^{\omega}d\varepsilon\frac{\varepsilon^{\beta}}{\varepsilon^2+a^2+E_{g0}^2}-2\int_0^{\omega}d\varepsilon\frac{a^2\varepsilon^{\beta}}{(\varepsilon^2+a^2+E_{g0}^2)^2}\}$$

We have

$$\int_0^{\omega}d\varepsilon\frac{\varepsilon^{\beta}}{\varepsilon^2+a^2+E_{g0}^2}=\frac{1}{2}(a^2+E_{g0}^2)^{(\beta-1)/2}B_{x_2}(\frac{\beta+1}{2},\frac{1-\beta}{2})$$

and

$$\int_0^{\omega}d\varepsilon\frac{\varepsilon^{\beta}}{[\varepsilon^2+a^2+E_{g0}^2]^2}=\frac{1}{2}(a^2+E_{g0}^2)^{(\beta-3)/2}B_{x_2}(\frac{\beta+}{2},\frac{3-\beta}{2})$$

here $x_2=\dfrac{\omega^2}{\omega^2+a^2+E_{g0}^2}$.

With these results of integration, we can get

$$\frac{\partial L(\omega,T_c)}{\partial T_c}=\frac{2N_0}{E_F^{\beta}}\sum_{n=0}^{\infty}\{(a^2+E_{g0}^2)^{(\beta-1)/2}B_{x_2}(\frac{\beta+1}{2},\frac{1-\beta}{2})-2a^2(a^2+E_{g0}^2)^{(\beta-3)/2}B_{x_2}(\frac{\beta+1}{2},\frac{3-\beta}{2})\} \tag{5.60}$$

Substitution of Eq.(5.59) and Eq.(5.60) into Eq.(5.12), we can find the s-wave isotope exponent with a pseudogap as

$$\alpha_{sp}=\frac{-\frac{1}{4}\omega_p^{\beta+1}\tanh(\frac{\sqrt{\omega_p^2+E_{g0}^2}}{2T_c})}{T_c\sqrt{\omega_p^2+E_{g0}^2}\sum_{n=0}^{\infty}\{f_{sp}(\omega_p)+\frac{V_{e0}}{V_{p0}}[\frac{1-V_{p0}L_p+2V_{p0}L_e}{1-V_{e0}L_e}]f_{sp}(\omega_e)\}} \tag{5.61}$$

where

$$f_{sp}(\omega)=(E_{g0}^2+a^2)^{\frac{\beta-1}{2}}B_{x_2}(\frac{\beta+1}{2},\frac{1-\beta}{2})-2a^2(E_{g0}^2+a^2)^{\frac{\beta-3}{2}}B_{x_2}(\frac{\beta+1}{2},\frac{3-\beta}{2}) \ .$$

In the case $E_{g0}=0$, Eq.(5.61) gives α of the s-wave superconductor without a pseudogap .

D-Wave without a Pseudogap

For a d-wave superconductor without a pseudogap, we must include the effect of the angular direction of momentum. Inserting a power law singularity DOS and the condition for d-wave and pseudogap in Eq.(5.9), we get

$$L(\omega,T_c) = \frac{N_0}{2\pi}\int_0^{2\pi} d\theta\psi_\eta^2(\theta)\int_0^{\omega}\frac{d\varepsilon}{\varepsilon}(\frac{\varepsilon}{E_F})^{\beta}\tanh(\frac{\varepsilon}{2T_c})$$

$$= <\psi_\eta^2(\theta)>\frac{N_0}{E_F^{\beta}}\int_0^{\omega} d\varepsilon\, \varepsilon^{\beta-1}\tanh(\frac{\varepsilon}{2T_c}) \qquad (5.62)$$

For d-wave case, $\psi_\eta(\theta) = \cos(2\theta)$ then we get $<\psi_\eta^2(\theta)> = \frac{1}{2}$.

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial \omega}$ and $\frac{\partial L}{\partial T_c}$ and obtain

$$\frac{\partial L(\omega,T_c)}{\partial \omega} = \frac{N_0}{2E_F^{\beta}}\tanh(\frac{\omega}{2T_c})\,\omega^{\beta-1} \qquad (5.63)$$

and

$$\frac{\partial L(\omega,T_c)}{\partial T_c} = \frac{2N_0}{T_c}\{-(\frac{\omega}{E_F})^{\beta}\tanh(\frac{\omega}{2T_c}) + \beta T_c^{\beta}(\frac{2}{E_F})^{\beta}\sum_{n=0}^{\infty}(\pi(n+1/2))^{\beta-1}B_{x_1}(\frac{\beta+1}{2},\frac{1-\beta}{2})\}$$

(5.64)

Substitution of Eq.(5.63) and Eq.(5.64) into Eq.(5.12), we find the d-wave isotope exponent without a pseudogap as

$$\alpha_{dp0} = \frac{\frac{1}{2}\omega_p^{\beta}\tanh(\frac{\omega_p}{2T_c})}{\{f_{dp0}(\omega_p) + \frac{V_{e0}}{V_{p0}}[\frac{1-V_{p0}L_p + 2V_{p0}L_e}{1-V_{e0}L_e}]\, f_{dp0}(\omega_e)\}} \qquad (5.65)$$

where $f_{dp0}(\omega) = \omega^{\beta}\tanh(\frac{\omega}{2T_c}) - 2\beta T_c\sum_{n=0}^{\infty} a^{\beta-1}B_{x_1(\omega)}(\frac{\beta+1}{2},\frac{1-\beta}{2})$.

Eq.(5.65) is the same as Eq.(5.57) that is the isotope exponent of s-wave without pseudogap, but

$L(\omega,T_c)$ of d-wave $=(1/2)$ $L(\omega,T_c)$ of s-wave (5.66)

D-Wave with a Pseudogap

For a d-wave superconductor with a pseudogap, we must include the effect of the angular direction of momentum in pseudogap and the condition of d-wave. Inserting a power law singularity DOS and condition of d-wave and pseudogap in Eq.(5.9), we can get

$$L(\omega,T_c)=\frac{N_0}{2\pi}\int_0^{2\pi}d\theta\cos^2(2\theta)\int_0^{\omega}d\varepsilon\frac{(\varepsilon/E_F)^{\beta}}{\sqrt{\varepsilon^2+E_{g0}^2\cos^2(2\theta)}}\tanh\left(\frac{\sqrt{\varepsilon^2+E_{g0}^2\cos^2(2\theta)}}{2T_c}\right) \tag{5.67}$$

$$=\frac{4N_0T_c}{\pi}\int_0^{\omega}d\varepsilon\int_0^{2\pi}d\theta\sum_{n=0}^{\infty}\frac{(\varepsilon/E_F)^{\beta}}{E_{g0}^2+\varepsilon^2+a^2+[\varepsilon^2+a^2]\tan^2(2\theta)}$$

We get

$$L(\omega,T_c)=\frac{2N_0T_c}{E_F^{\beta}}\sum_{n=0}^{\infty}\{\frac{1}{2}(a^2+E_{g0}^2)^{\frac{\beta-1}{2}}B_x(\frac{\beta+1}{2},\frac{1-\beta}{2})$$

$$+\sum_{k=1}^{\infty}[(\frac{\prod_{p=1}^{k}(2p-1)}{\prod_{p=0}^{k}(2p+2)})E_{g0}^{2k}(a^2+E_{g0}^2)^{\frac{\beta-2k-1}{2}}B_x(\frac{\beta+1}{2},\frac{1+2k-\beta}{2})\}\ .$$

To find the isotope exponent, we must calculate $\frac{\partial L}{\partial\omega}$ and $\frac{\partial L}{\partial T_c}$ and obtain

$$\frac{\partial L(\omega,T_c)}{\partial\omega}=\frac{4N_0T_c}{\pi}\int_0^{2\pi}d\theta\sum_{n=0}^{\infty}\frac{(\varepsilon/E_F)^{\beta}}{E_{g0}^2+\varepsilon^2+a^2+[\varepsilon^2+a^2]\tan^2(2\theta)}$$

$$=\frac{4N_0T_c}{E_{g0}^2}(\frac{\omega}{E_F})^{\beta}\sum_{n=0}^{\infty}(1-\sqrt{\frac{\omega^2+a^2}{\omega^2+a^2+E_{g0}^2}}) \tag{5.68}$$

and

$$\frac{\partial L(\omega,T_c)}{\partial T_c}=\frac{4N_0}{E_{g0}^2}\sum_{n=0}^{\infty}\int_0^{\omega}d\varepsilon(\frac{\varepsilon}{E_F})^{\beta}[1-\sqrt{\frac{\varepsilon^2+a^2}{\varepsilon^2+a^2+E_{g0}^2}}-\frac{a^2E_{g0}^2}{\sqrt{(\varepsilon^2+a^2)(\varepsilon^2+a^2+E_{g0}^2)}}]\ .$$

Consider the integration

$$\int_0^{\omega} d\varepsilon\, \varepsilon^{\beta} (1-\sqrt{\frac{\varepsilon^2+a^2}{\varepsilon^2+a^2+E_{g0}^2}}) = \int_0^{\omega} d\varepsilon \varepsilon^{\beta} \{\frac{E_{g0}^2}{2(\varepsilon^2+a^2+E_{g0}^2)} + \sum_{k=1}^{\infty} \frac{\prod_{p=1}^{k}(2p-1)}{\prod_{p=0}^{k}(2p+2)} \frac{E_{g0}^{2k+2}}{(\varepsilon^2+a^2+E_{g0}^2)^{k+1}}\}$$

$$= \frac{E_{g0}^2}{4}(a^2+E_{g0}^2)^{\frac{\beta-1}{2}} B_{x_2}(\frac{\beta+1}{2},\frac{1-\beta}{2}) + \frac{1}{2}\sum_{k=1}^{\infty} \frac{\prod_{p=1}^{k}(2p-1)}{\prod_{p=0}^{k}(2p+2)} E_{g0}^{2k+2}(a^2+E_{g0}^2)^{\frac{\beta-2k-1}{2}} B_{x_2}(\frac{\beta+1}{2},\frac{1+2k-\beta}{2})$$

(5.69)

and

$$\int_0^{\omega} d\varepsilon \frac{\varepsilon^{\beta}}{\sqrt{\varepsilon^2+a^2}(\varepsilon^2+a^2+E_{g0}^2)^{3/2}} = \int_0^{\omega} d\varepsilon \varepsilon^{\beta} \{\frac{1}{(\varepsilon^2+a^2+E_{g0}^2)^2} + \sum_{k=1}^{\infty} \frac{\prod_{p=1}^{k}(2p-1)}{\prod_{p=1}^{k}(2p)} \frac{E_{g0}^{2k}}{(\varepsilon^2+a^2+E_{g0}^2)^{k+2}}\}$$

$$= \frac{1}{2}(a^2+E_{g0}^2)^{\frac{\beta-3}{2}} B_{x_2}(\frac{\beta+1}{2},\frac{3-\beta}{2}) + \frac{1}{2}\sum_{k=1}^{\infty} \frac{\prod_{p=1}^{k}(2p-1)}{\prod_{p=1}^{k}(2p)} E_{g0}^{2k}(a^2+E_{g0}^2)^{\frac{\beta-2k-3}{2}} B_{x_2}(\frac{\beta+1}{2},\frac{3+2k-\beta}{2})$$

(5.70)

Substitution of Eqs.(5.68), (5.69), and Eq.(5.70) into Eq.(5.12), we find the d-wave isotope exponent with a pseudogap as

$$\alpha_{dp} = \frac{\frac{\omega_p^{\beta+1}}{E_{g0}^2}\sum_{n=0}^{\infty}(\sqrt{\frac{\omega_p^2+a^2}{\omega_p^2+a^2+E_{g0}^2}}-1)}{\{f_{dp}(\omega_p)+\frac{V_{e0}}{V_{p0}}[\frac{1-V_{p0}L_p+2V_{p0}L_e}{1-V_{e0}L_e}]f_{dp}(\omega_e)\}} \tag{5.71}$$

where $$f_{dp}(\omega)=\sum_{n=0}^{\infty}\{\frac{E_F^{\beta}}{N_0T_c}L(\omega,T_c)-a^2(a^2+E_{g0}^2)^{\frac{\beta-3}{2}}B_x(\frac{\beta+1}{2},\frac{3-\beta}{2})$$

$$-a^2(\frac{\prod_{p=1}^{k}(2p-1)}{\prod_{p=1}^{k}2p})E_{g0}^{2k}(a^2+E_{g0}^2)^{\frac{\beta-2k-3}{2}}B_x(\frac{\beta+1}{2},\frac{3+2k-\beta}{2})]\}$$

and $$L(\omega,T_c)=\frac{N_0T_c}{E_F^{\beta}}\sum_{n=0}^{\infty}\{\frac{1}{2}(a^2+E_{g0}^2)^{\frac{\beta-1}{2}}B_x(\frac{\beta+1}{2},\frac{1-\beta}{2})$$

$$+\sum_{k=1}^{\infty}[(\frac{\prod_{p=1}^{k}(2p-1)}{\prod_{p=0}^{k}(2p+2)})E_{g0}^{2k}(a^2+E_{g0}^2)^{\frac{\beta-2k-1}{2}}B_x(\frac{\beta+1}{2},\frac{1+2k-\beta}{2})\}\ .$$

In case $E_{g0}=0$, Eq.(5.71) gives α of a d-wave superconductor without a pseudogap having the same form as that of s-wave without a pseudogap for both cases of the constant DOS and VHS DOS.

CHAPTER VI

DISCUSSION AND CONCLUSIONS

The purpose of this work is to explain the unusual isotope coefficients of cuprates by considering the influence of the pseudogap and the phononic and the electronic interactions in weak-coupling limit. Exact analytic expressions for the isotope exponent (α) for the s-wave and d-wave pairing symmetry with constant, VHS and power law density of states are derived .

The equations of the isotope exponent are so complicated to understand. In order to understand those formula , the numerical calculation is used.

The computer program is written by using the iteration method, numerical integration and numerical summation. To solve the equation, the Newton iteration method is defined as

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

where f(x) is any function that f(x)=0 and

$$f'(x) = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}} \quad .$$

We also compare our calculation of all cases to the experimental data of $La_{2-x}Ba_xCuO_4$ (●), $La_{2-x}Sr_xCuO_4$(■) (Crawford et al., 1990), and $(Y_{1-x-y}Pr_xCa_y)Ba_2Cu_3O_{7-\delta}$ (□), $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$ (□), $YBa_2(Cu_{1-z}Zn_z)_3O_{7-\delta}$ (*)(Soerensen and Gygax, 1995), and $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$ (+) (Franck et al., 1991), and $YBa_{2-x}La_xCu_3O_{7-\delta}$ (Δ) (Bornemann and Morris, 1991) .

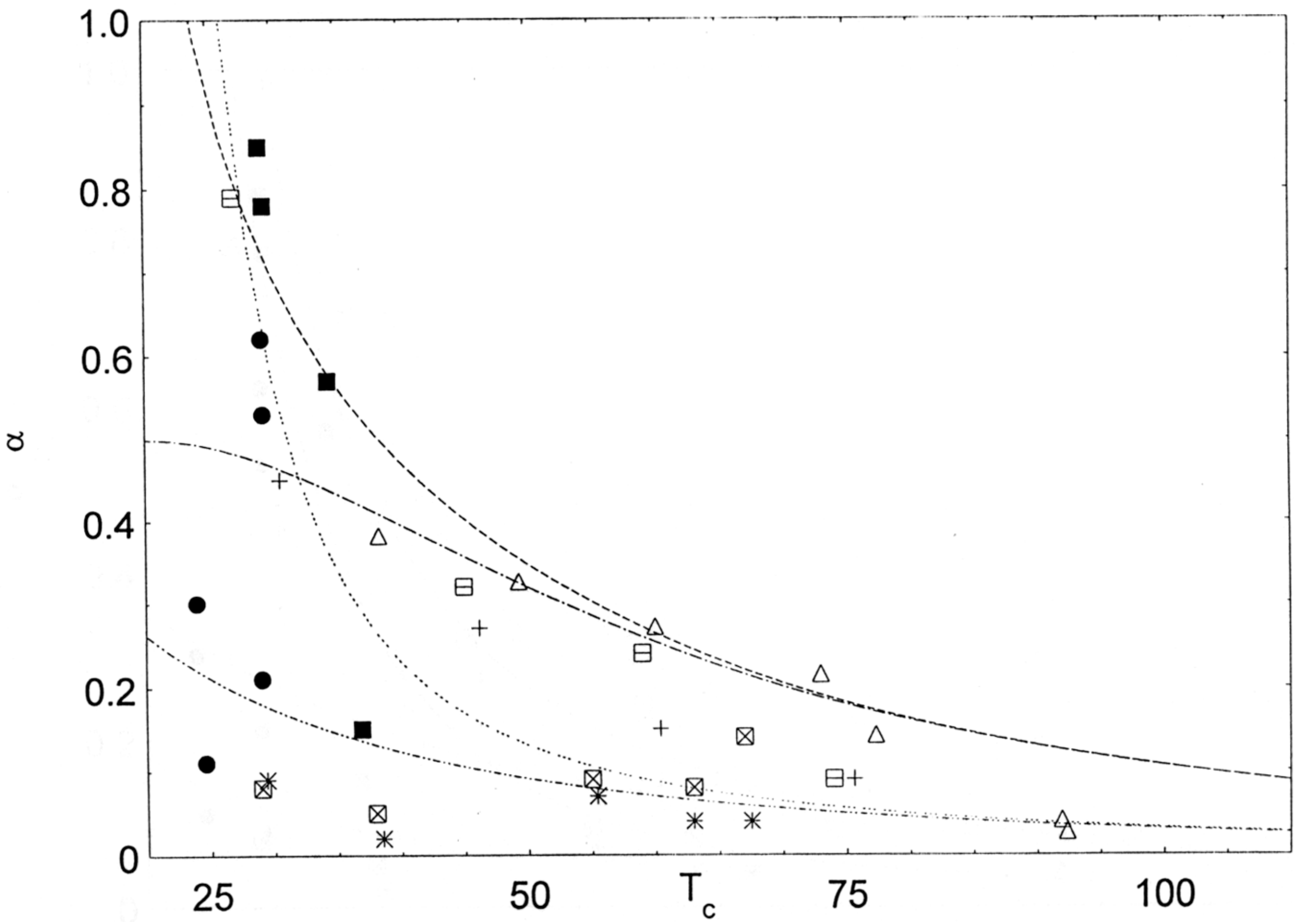
Constant Density of States

By computing Eq.(5.10), Eq.(5.21) and Eq.(5.33) numerically, we plot the isotope exponent α against T_c for the s-wave and d-wave cases. The influence of pseudogap on the isotope exponent for the s-wave pairing is shown in Figure(6.1) and that for the d-wave pairing is shown in Figure(6.2) .

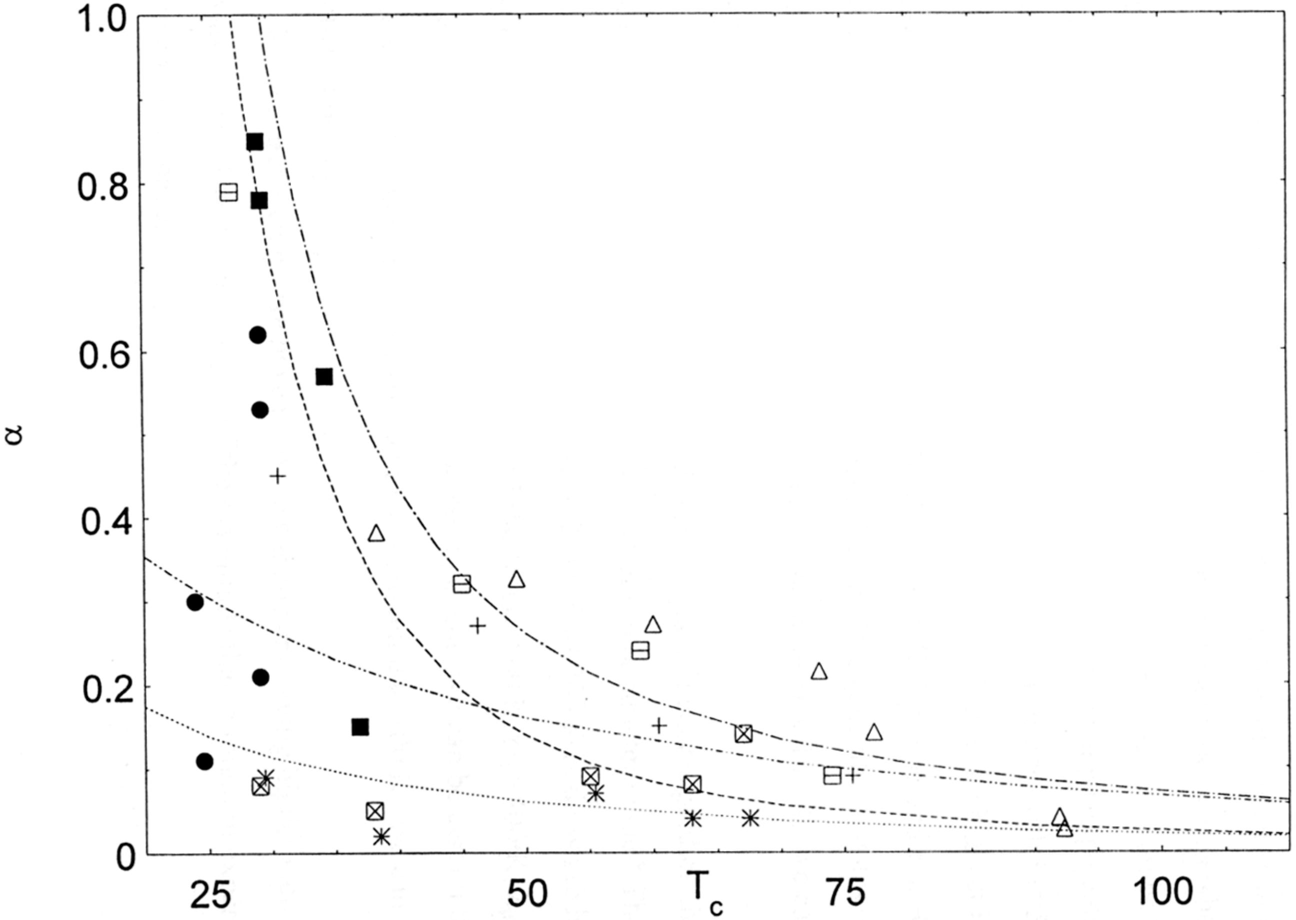
In Figure(6.1), we have shown for all s-wave cases with various values of ω_p, ω_e , λ_p and E_{g0}, here we define that λ_p=N_0V_{p0} and λ_e=N_0V_{e0} . All curves shown that the isotope exponent decreases when the T_c of doped cuprate increases. In low-critical temperature region the isotope exponent is higher than conventional value of 1/2, and in the high-T_c region the isotope exponent has small almost zero values (depending on the parameters). When ω_p=500 K, ω_e =400 K, λ_p=0.3 and E_{g0} =50 K is shown it has the highest isotope exponent and ω_p=500 K, ω_e =400 K, λ_p=0.2 and E_{g0} =0 K is shown the smallest isotope exponent. This mean that if we vary the value of λ_p between 0.2 to 0.3 and E_{g0} between 0 to 50 K we can fit every experimental data.

In Figure(6.2), we have shown the d-wave cases. All curves show the similar behavior as the s-wave cases but they are different in values. The graph with ω_p=700 K, ω_e =650 K, λ_p=0.4 and E_{g0} =150 K is shown to have the highest isotope exponent and the graph with ω_p=500 K, ω_e =400 K, λ_p=0.35 and E_{g0} =0 K is shown to have the smallest isotope exponent. We can therefore assume that if we vary the value of λ_p between 0.4 to 0.35 and E_{g0} between 0 to 150 K, we can fit every experimental data.

In the d-wave cases, we have used the higher values of parameter than in the s-wave cases. But the values of E_{g0} is not of the same magnitude that found in experiments and the value of λ_p is high almost beyond the weak-coupling limit.



Figure(6.1) Plot of the isotope exponent α versus T_c(in K) for the s-wave pairing with influence of constant DOS and ω_p=500K, ω_e=400K, with various values of λ_p and E_{go} : (– – – –) λ_p =0.3, E_{g0}=50K , (—·—·) λ_p =0.3, E_{g0}= 0K, (·· ··· ··) λ_p =0.2, E_{g0}=120K, and (–··–··) λ_p =0.2, E_{g0}=0K. We compare our calculation with the experimental data of $La_{2-x}Ba_xCuO_4$ (●), $La_{2-x}Sr_xCuO_4$(■) (Crawford et al., 1990), and $(Y_{1-x-y}Pr_xCa_y)Ba_2Cu_3O_{7-\delta}$ (⊠), $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$ (⊟), $YBa_2(Cu_{1-z}Zn_z)_3O_{7-\delta}$ (*)(Soerensen and Gygax, 1995), and $(Y_{1-x}Pr_x)Ba_2Cu_3O_{7-\delta}$ (+) (Franck et al., 1991), and $YBa_{2-x}La_xCu_3O_{7-\delta}$ (Δ) (Bornemann and Morris, 1991) .



Figure(6.2) Plot of the isotope exponent α versus T_c(in K) for the d-wave pairing with influence of constant DOS with various values of ω_p, ω_e, λ_p and E_{go} : (– – –) λ_p =0.35, ω_p=500K, ω_e=400K, E_{g0}=250K, (·······) λ_p =0.35, ω_p=500K, ω_e=400K, E_{g0}= 0K, (–··—·) λ_p =0.4, ω_p=700K, ω_e=650K, E_{g0}= 0K, and (—· —·) λ_p =0.4, ω_p=700K, ω_e=650K, E_{g0}=150K.

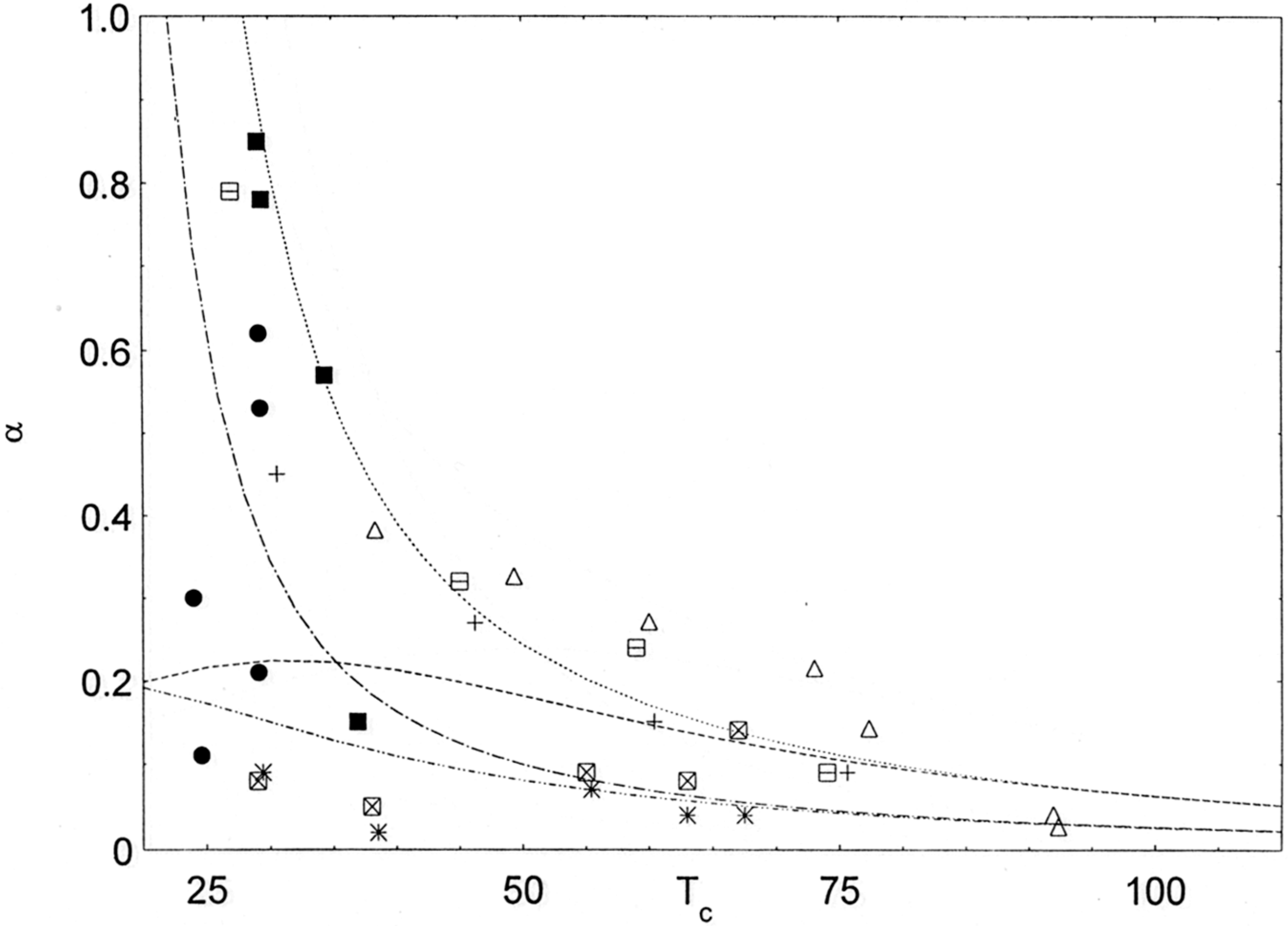
Van Hove Singularity Density of States

By computing Eq.(5.10), Eq.(5.42), and Eq.(5.52) numerically, we plot the isotope exponent α against T_c for the s-wave and d-wave cases. The influence of pseudogap on the isotope exponent for the s-wave pairing is shown in Figure(6.3) and that for the d-wave pairing is shown in Figure(6.4) .

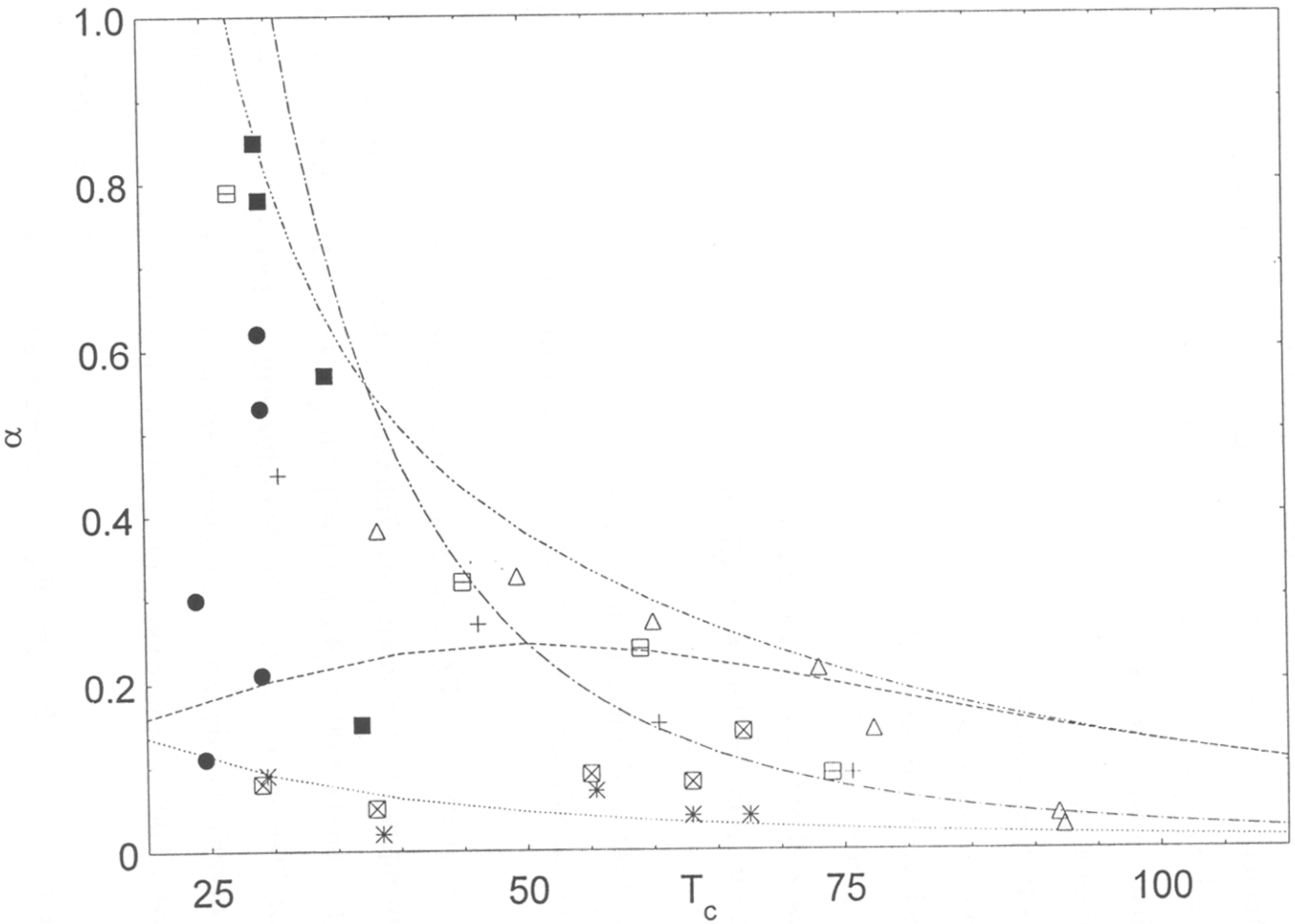
In Figure(6.3), we have shown for all s-wave cases with various values of ω_p, ω_e , λ_p and E_{g0} . All curves show that the isotope exponent decreases when the T_c of doped cuprate increases. In the low-T_c region the isotope exponent can be higher than conventional value of 1/2, and in the high-T_c region the isotope exponent has small almost zero values (depending on the parameters). The graph with E_F=5580 K, ω_p=500 K, ω_e =400 K, λ_p=0.08 and E_{g0} =100 K is shown to have the highest isotope exponent and that with E_F=5580 K, ω_p=500 K, ω_e =400 K, λ_p=0.06 and E_{g0} =0 K is shown to have the smallest isotope exponent. For the VHS density of states, if we vary the value of λ_p between 0.06 to 0.08 and E_{g0} between 0 to 100 K, we can fit every experimental data.

In Figure(6.4), we have shown all d-wave cases. All curves predict the same behavior as in the s-wave cases but they are different in parameter values. The graph with E_F=5580 K, ω_p=700 K, ω_e =650 K, λ_p=0.2 and E_{g0} =700 K is shown to have the highest isotope exponent and that with E_F=5580 K, ω_p=500 K, ω_e =400 K, λ_p=0.1 and E_{g0} =0 K is shown to have the smallest isotope exponent. We can be certain that if we vary the value of λ_p between 0.1 to 0.2 and E_{g0} between 0 to 700 K, we can fit every experimental data.

In the d-wave cases, we have used the parameters having higher values than the s-wave cases. The value of E_{g0} is of the magnitude that is found in experiments (Suzuki and Watanabe, 2000) .



Figure(6.3) Plot of the isotope exponent α versus T_c(in K) for the s-wave pairing with influence of VHS DOS and E_F=5580K, ω_p=500K, ω_e=400K with various values of λ_p and E_{go} : (–-—) λ_p =0.06, E_{g0}=100K, (–··—·) λ_p =0.06, E_{g0}= 0K, (·······) λ_p =0.08, E_{g0}= 100K, and (–––-) λ_p =0.08, E_{g0}=0K.



Figure(6.4) Plot of the isotope exponent α versus T_c(in K) for the d-wave pairing with influence of VHS DOS and E_F=5580K, ω_p=500K, ω_e=400K with various values of λ_p and E_{go} : (–··–) λ_p =0.2, E_{g0}=100K, (—·—) λ_p =0.1, E_{g0}= 700K, (·······) λ_p =0.1, E_{g0}= 0K, and (– – – –) λ_p =0.2, E_{g0}=0K.

Power Law Density of States

By computing Eq.(5.10), Eq.(5.61), and Eq.(5.71) numerically, we plot the isotope exponent α against T_c for the s-wave and d-wave cases. The influence of pseudogap on the isotope exponent for the s-wave pairing is shown in Figure(6.5) and Figure(6.7) and that for the d-wave pairing is shown in Figure(6.6) and Figure(6.8).

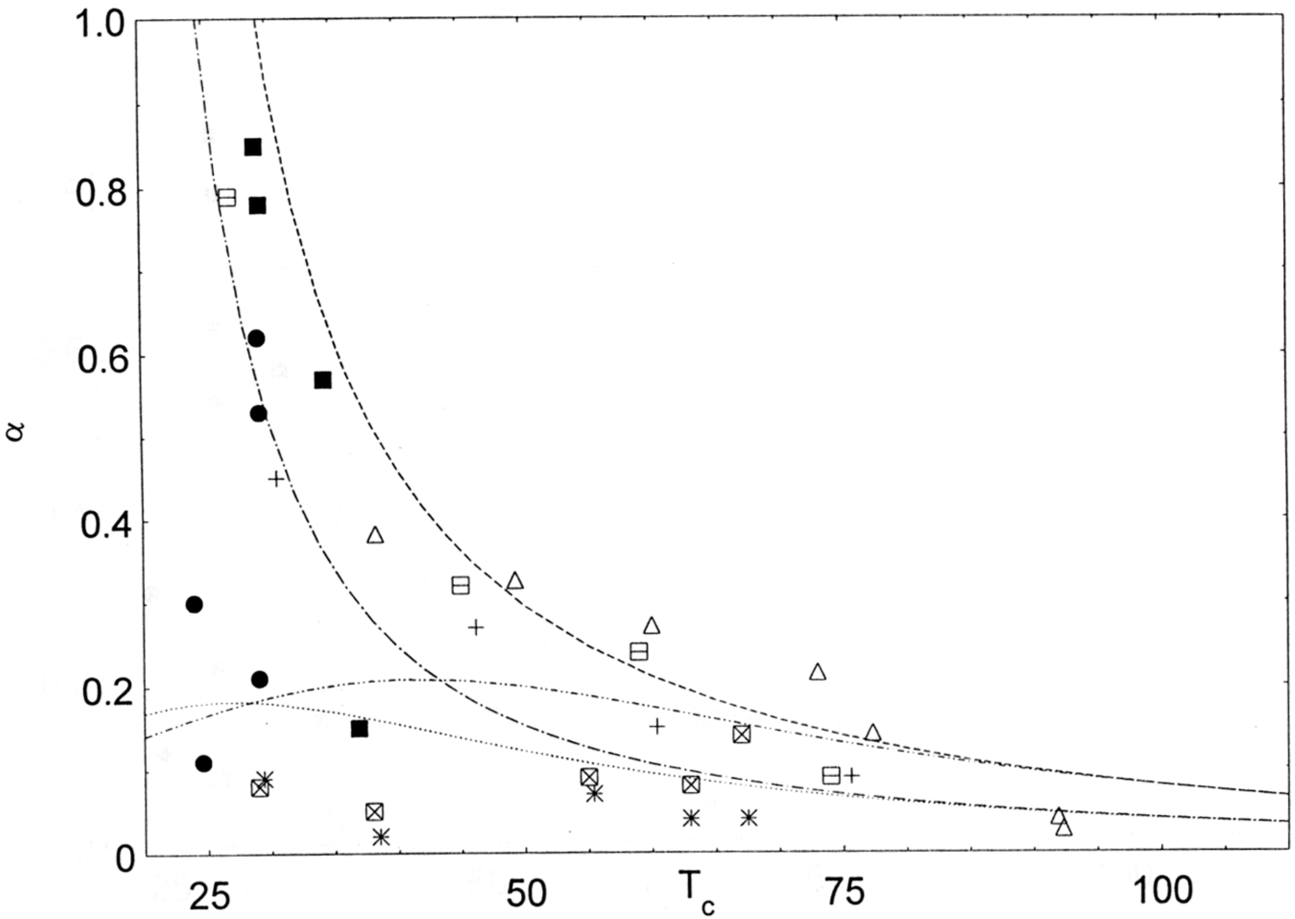
In Figure(6.5), we have shown for all s-wave cases with various values of ω_p, ω_e, λ_p and E_{g0}. All curves show that the isotope exponent decrease when the T_c of doped cuprate increases. In the low-T_c region the isotope exponent can be higher than the conventional value of 1/2, and in the high-T_c region the isotope exponent shows the small almost zero values (depending on the parameters). The graph with E_F=5580 K, ω_p=500 K, ω_e =400 K, λ_p=0.1, β= -0.3 and E_{g0} =100 K is shown to have the highest isotope exponent and that with E_F=5580 K, ω_p=500 K, ω_e =400 K, λ_p=0.08, β=-0.3 and E_{g0} =0 K is shown to have the smallest isotope exponent. Thus for the s-wave, if we vary the value of λ_p between 0.08 to 0.1 and E_{g0} between 0 to 100 K, we can fit every experimental data.

The effect of β on isotope exponent is shown in Figure(6.7) for the s-wave cases. Graphs with values of β between -0.2 to -0.5 give the highest value of α and α increases when E_{g0} increases.

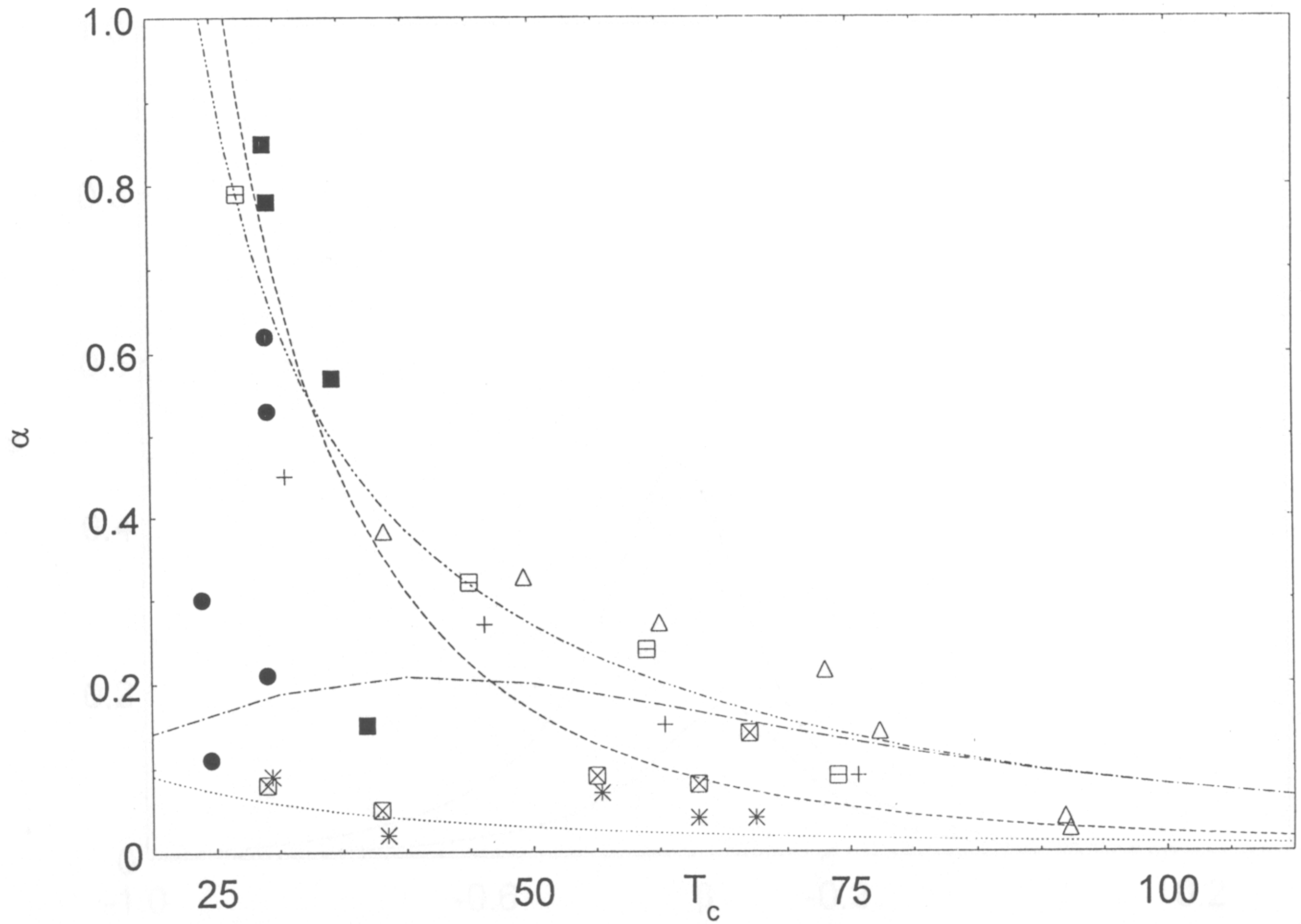
In Figure(6.6), we have shown all d-wave cases. All curves show the similar behavior to the s-wave cases but they have different parameters. The graph with E_F=5580 K, ω_p=500 K, ω_e =400 K, λ_p=0.1, β=-0.3 and E_{g0} =700 K is shown to have the highest isotope exponent and that with E_F=5580 K, ω_p=500 K, ω_e =400 K, λ_p=0.1, β=-0.3 and E_{g0} =0 K is shown to have the smallest isotope exponent. Thus in this case, if we vary the value of λ_p between 0.1 to 0.2 and E_{g0} between 0 to 700 K, we can fit every experimental data.

In the d-wave cases, we use the parameter having higher values than in the s-wave cases. The value of E_{g0} used is of the same magnitude as that found in experiments .

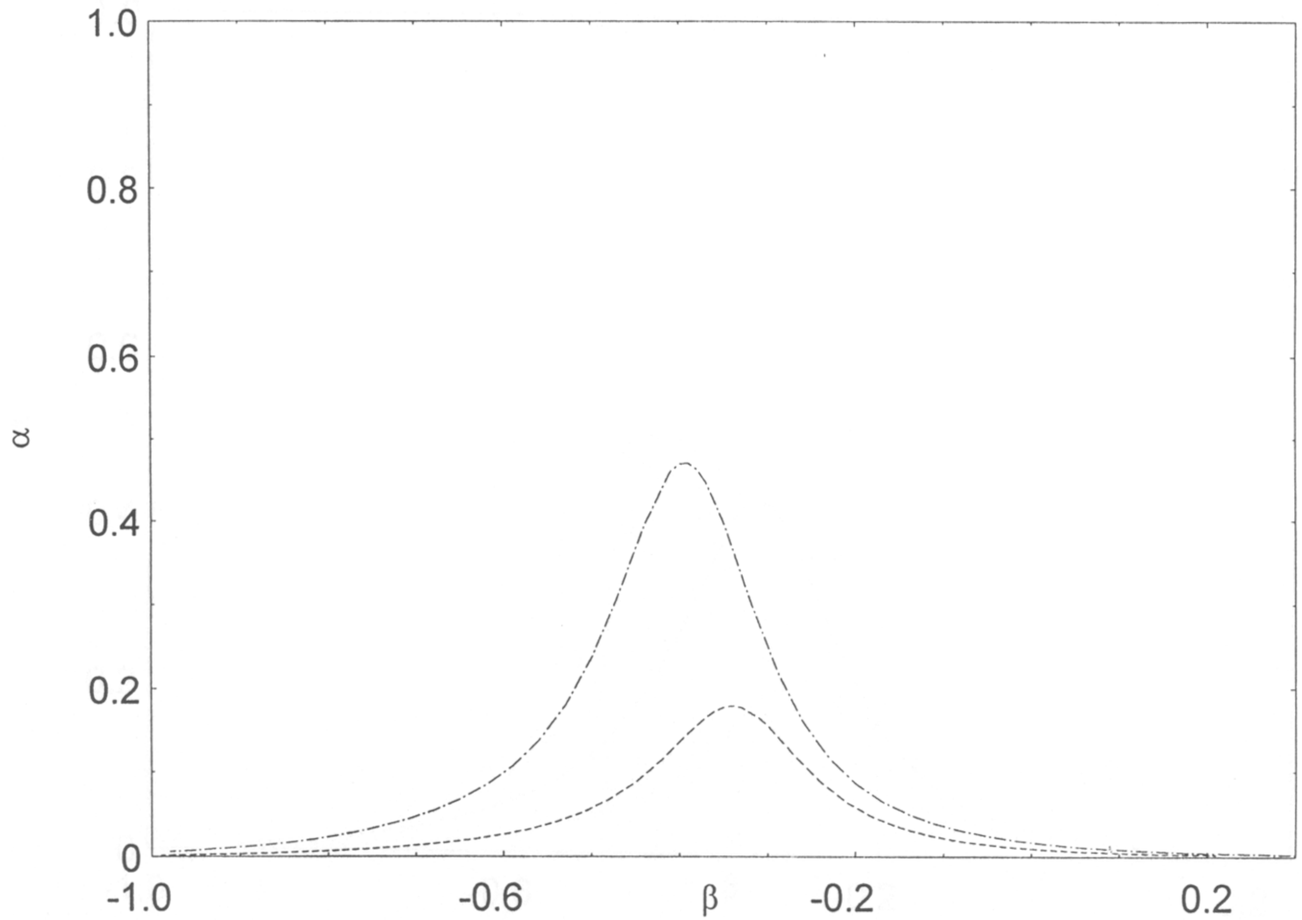
The effect of β on isotope exponent is shown in Figure(6.8) for the d-wave cases. We find that when of β varies between -0.2 to -0.5, it gives the highest values of α and α increases when E_{g0} increases in the same as the s-wave cases.



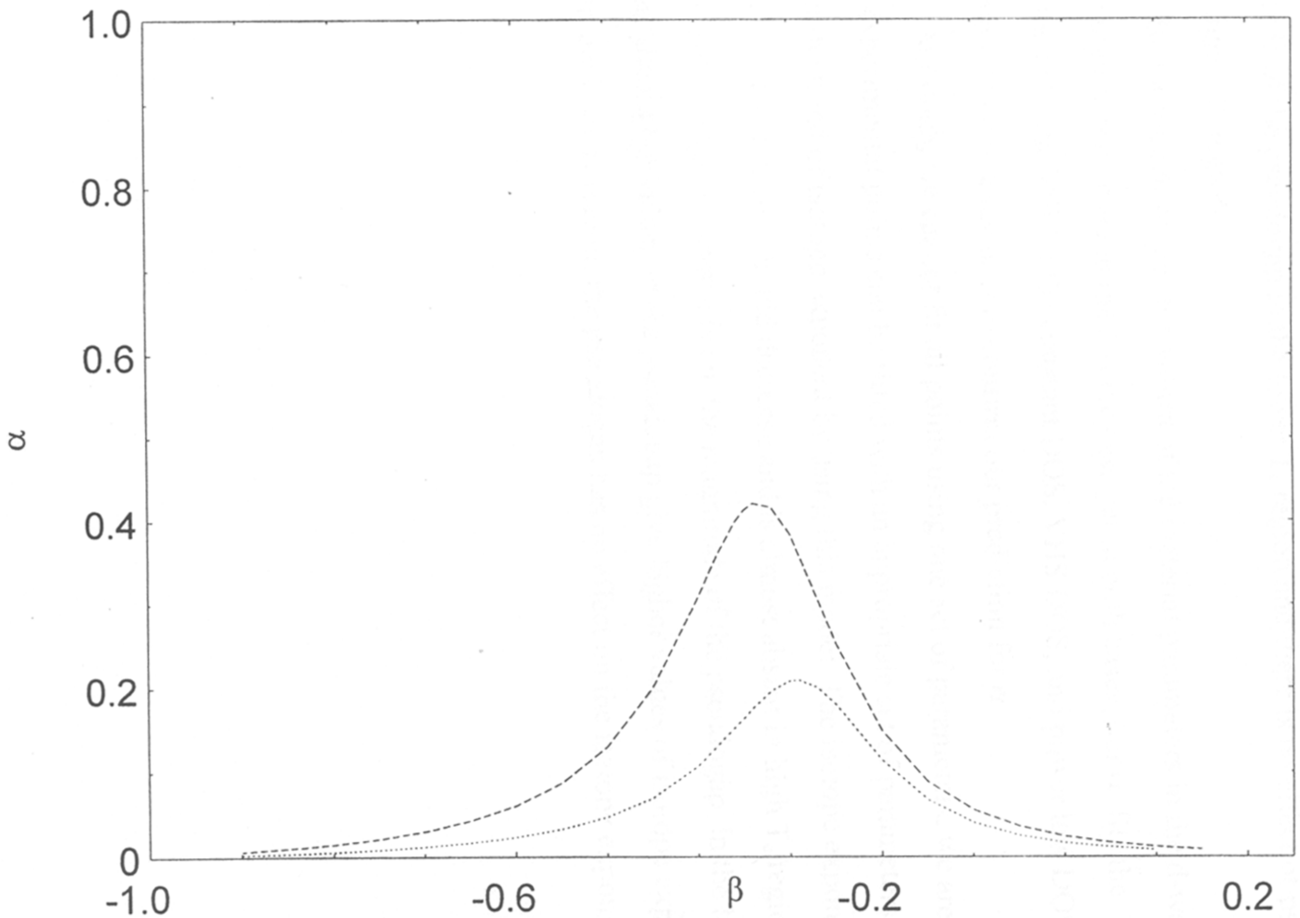
Figure(6.5) Plot of the isotope exponent α versus T_c(in K) for the s-wave pairing with influence of power law DOS and E_F=5580K, β=-0.3 with various values of ω_p,ω_e,λ_p and E_{go} : (–·–·) λ_p =0.08, ω_p=500K, ω_e=400K, E_{g0}=100K , (······) λ_p =0.08, ω_p=500K, ω_e=400K, E_{g0}= 0K, (– – – –) λ_p =0.1, ω_p=500K, ω_e=400 K, E_{g0}= 100K, and (–··–·) λ_p =0.1, ω_p=500 K, ω_e=400K, E_{g0}=0K.



Figure(6.6) Plot of the isotope exponent α versus T_c(in K) for the d-wave pairing with influence of power law DOS and E_F=5580K, β=-0.3, ω_p=500K, ω_e=400K with various values of λ_p and E_{go} : (—··—) λ_p =0.2, E_{g0}=100K , (—·—·) λ_p =0.2, E_{g0}= 0K,(– – – –) λ_p =0.1, E_{g0}= 700K, and (·······) λ_p =0.1, E_{g0}=0K.



Figure(6.7) Plot of the isotope exponent α versus β for the s-wave pairing with influence of power law DOS and E_F=5580K,T_c=40K,λ_p =0.08, ω_p=500K, ω_e=400K with various values of E_{go} : (– – –) E_{g0}=0K, (–· –·) E_{g0}= 100K.



Figure(6.8) Plot of the isotope exponent α versus β for the d-wave pairing with influence of power law DOS and E_F=5580K,T_c=40K,λ_p =0.2, ω_p=500K, ω_e=400K with various values of E_{go} : (······) E_{g0}=0K, (– – – –) E_{g0}= 100K.

Conclusions

We have investigated the effect of the pseudogap on the isotope exponent in the s- and d-wave pairing states in the weak-coupling limited. Our formulas can explain the unusual isotope effect of cuprates having both smaller and higher values than 0.5 . The magnitude of the isotope exponent is proportional to the magnitude of the pseudogap in the lower T_c region and there is no effect of pseudogap in the higher T_c region.

In our model, we use the values of the material parameters in the d-wave case having higher than those in the s-wave case yet in both cases, our α fits the experimental data well for the constant DOS, VHS DOS, and power law DOS. So we need more experimental data to confirm our prediction for α .

Although, we cannot fit all points using one set of parameters, we are sure that every experimental points can be fitted with an appropriate set of parameters. We can predict the trend of isotope exponent by using this model. The isotope exponent of a high-T_c superconductor should decrease and is almost absent in high T_c region and for the low T_c region it depends on the magnitude of the pseudogap. In the low T_c region, the higher values of the pseudogap give higher values of isotope exponent. And in the high T_c region, the pseudogap has no effect on the isotope exponent.

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APPENDIX

APPENDIX

Evaluation of Frequency Sums

The frequency sum in Eq.(2.8) is typical of those occurring in many-body physics. This equation had been done by Fetter and Walecka (1971).

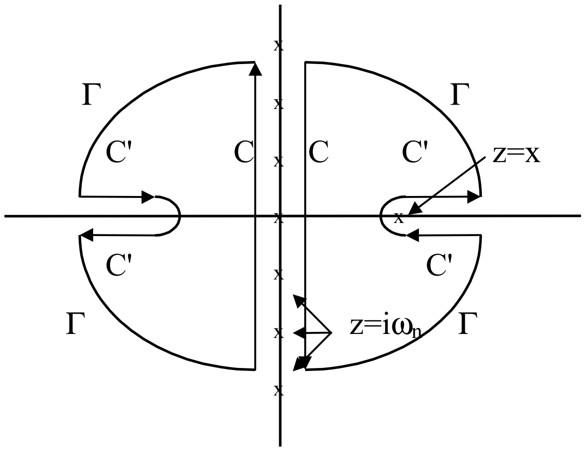

Fig.(A.1) Coutour for evaluation of frequency sums (Fetter and Walecka,1971) .

For definiteness, consider the case of boson, where the sum is of the form

$$\sum_n e^{i\omega_n \eta}(i\omega_n - x)^{-1} \tag{A.1}$$

with $\omega_n = 2n\pi / \beta\eta$ and β=1/k_bT. Eq.(A.1) is not absolute convergent, for it would diverge logarithmically without the convergence factor ; η must therefore remain positive unit after the sum is evaluated.

The most direct approach is to use contour integration, which requires a meromorphic function with poles at even integers. One possible choice is

$\beta\eta(e^{\beta\eta z}-1)^{-1}$, whose pole occur at $z = 2n\pi i / \beta\eta = i\omega_n$, each with unit residue. If C is a contour encircling the imaginary axis in the positive sense (Fig.(A.1)), then the contour integral

$$\frac{\beta\eta}{2\pi i}\int_C \frac{dz}{e^{\beta\eta z}-1}\frac{e^{\eta z}}{z-x} \tag{A.2}$$

exactly reproduces the sum in Eq.(A.1), because the integrand has an infinite sequence of simple poles at $i\omega_n$ with residue $\frac{e^{i\omega_n\eta}}{\beta\eta(i\omega_n - x)}$. Deform the contour to C' and Γ shown in Fig.A.1 . If $|z| \to \infty$ along a ray with Re z >0, then the integrand is of order $\frac{\exp[-(\beta\eta-\eta)\,\mathrm{Re}\,z]}{|z|}$; if $|z| \to \infty$ along a ray with Re z<0, then the integrand is of order $\frac{\exp(\eta\,\mathrm{Re}\,z)}{|z|}$. Since $\beta\eta > \eta > 0$, Jordan's lemma shows that the contributions of the large arcs Γ vanish and we are left with the integrals along C'

$$\sum_n \frac{e^{i\omega_n\eta}}{i\omega_n - x} = \frac{\beta\eta}{2\pi i}\int_{C'} \frac{dz}{e^{\beta\eta z}-1}\frac{e^{\eta z}}{z-x} \tag{A.3}$$

The only singularity included in C' is a simple pole at z=x, and Cauchy's theorem yields

$$\lim_{\eta\to 0}\sum_{n\,\mathrm{even}} \frac{e^{i\omega_n\eta}}{i\omega_n - x} = \frac{-\beta\eta}{e^{\beta\eta x}-1} \tag{A.4}$$

where the minus sign arises from the negative sense of C', and it is now permissible to let $\eta \to 0$. This derivation exhibits the essential role of the convergence factor. Although the function $\frac{-\beta\eta}{e^{-\beta\eta z}-1}$ also has simple poles at $z=i\omega_n$ with unit residue, the contributions from Γ would diverge in this case, thus preventing the deformation from C to C' .

A similar analysis may be give for fermions, where $\omega_n = (2n+1)\pi / \beta\eta$. The function $\frac{-\beta\eta}{e^{\beta\eta z}+1}$ has simple poles at the odd integers z=iω_n with unit residue, and the series can be rewritten as

$$\sum_{n\,odd} \frac{e^{i\omega_n \eta}}{i\omega_n - x} = \frac{-\beta\eta}{2\pi i} \int_C \frac{dz}{e^{\beta\eta z}+1} \frac{e^{\eta z}}{z-x} \qquad (A.5)$$

where C is the same contour as in Fig.(A.1) . Jordan's lemma again allows the contour deformation from C to C' because $\beta\eta > \eta > 0$, and the simple pole at z=x yields

$$\lim_{\eta \to 0} \sum_{n\,odd} \frac{e^{i\omega_n \eta}}{i\omega_n - x} = \frac{\beta\eta}{e^{\beta\eta x}+1} \qquad (A.6)$$

The two case can be combined in the single expression

$$\lim_{\eta \to 0} \sum_n \frac{e^{i\omega_n \eta}}{i\omega_n - x} = \mu \frac{\beta\eta}{e^{\beta\eta x}\ \mu\ 1} \qquad (A.7)$$

For general case, if we consider $\sum_n f(i\omega_n)$ by using the same process as above, we can get formula for fermion system as

$$T \sum_n f(i\omega_n) = -\oint \frac{dz}{2\pi i} n_F(z) f(z) \qquad (A.8)$$

where $n_F(z) = \frac{1}{e^{z/T}+1}$ is fermion distribution function and $\omega_n = (2n+1)\pi k_b T / \eta$.

For boson system, we get

$$T \sum_n f(i\omega_n) = \oint \frac{dz}{2\pi i} n_F(z) f(z) \qquad (A.9)$$

where $n_F(z) = \frac{1}{e^{z/T}-1}$ is boson distribution function and $\omega_n = n\pi k_b T / \eta$.

CURRICULUM VITAE

Mr.Pongkaew Udomsamuthirun was born on 1st June, 1969 in a small village of Samutprakan province, Thailand. He began his education in the Kaungsaotong primary school and the Samutprakan secondary school from 1974 to1981 and 1981 to 1987 respectively. After he finished the secondary school, he received the scholarship from the Institute for Promotion of Science and Teaching (IPST) to continue his education at department of Physics, Faculty of Science, Chulalongkorn University from1987 to1993 and he obtained the Bachelor of Science degree in 1990 and the Master of Science degree in1993. He started his career as a lecturer at the Department of Physics, Faculty of Science, Kasertsart University from 1993 to1995. From 1995 to present, he is a lecturer at Department of Physics, Faculty of Science, Srinakharinwirot University .