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## RESEARCH ARTICLE

### PHASE TRANSITION IN SUPERCONDUCTORS.

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#### Abstract

Phenomena of phase transition are a possible consequence of molecular interaction as in ordinary matter and superfluid systems, such as liquid, or electrons and nucleons interaction. These interactions are believed to be the cause of superconductivity of different types of materials and the Superfluidity of nuclear matter. It is also well known that the interaction between the electrons in the superconducting state may be different for different materials. Thus, for any high superconductor a possible type of electron-electron interaction may be used as a perturbation and the theory of second quantization may be used to study the possible phase transition in that material. According to the theory of second quantization, if a perturbation commutes with the rest of the Hamiltonian, it leads to a phase transition. Using theory of second quantization, a theoretical calculation has been performed to investigate the commutability in electron-phonon interaction, simultaneous existence of electron-phonon and coulomb interaction and exotic pairing as a characteristic of phase transition in a superconductor. Calculations show that the three interaction commutes with unperturbed Hamiltonian and may lead to a phase transition.

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#### Introduction:-

When temperature of frozen mercury is reduced below its critical temperature of about 4.2 K, its electrical resistance disappeared resulting in the flow of electrical current of the order of Amperes (Onnes, 1911). This disappearance of electrical resistance was termed superconductivity, and it opened up a new research field that was envisaged to usher in ideal electrical conductors. Later, it was found that a number of pure metals, alloys and doped semiconductors also become superconductors at very low temperatures, which are nowadays called conventional superconductors. In 1957, an acceptable microscopic theory for superconductivity, based on the concept of pairing of electrons of opposite spins and momenta (time-reversed states) near the Fermi surface, was given by Bardeen, Cooper and Schrieffer and is usually referred as BCS Theory (Bardeen, et al., 1957). The effective interaction between a pair of electrons (Cooper-pair) results from the virtual exchange of a phonon between the two electrons constituting the pair. Such an interaction is called electron-phonon interaction. The interaction is attractive when the energy difference between the electronic states involved is less than the phonon energy, and vice versa. The important contribution to the interaction energy is given by short rather than long wavelength phonon. The strength of this electron-phonon interaction also reaches peak when the electrons are in the states of equal and opposite momenta and of opposite spins.

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It is found that the critical temperature for transition to the superconducting state depends on the isotopic mass. This pointed to the possibility that the superconducting transition involved some kind of interaction with the crystal lattice. This supported the concept of electron-phonon interaction (Reynolds et al., 1950; Maxwell, 1950).

Bednorz and Muller (1986) discovered superconductivity in Lanthanum-based cuprateperovskite material, which had a transition temperature of 35 K.

Several theories have been advanced to describe the transition of materials from the normal state to the superconducting state, but their full understanding and simplification continue to emerge. In this work, three types of possible interactions between electrons in the crystal that are believed to cause transition to superconducting phase are explored theoretically using perturbation theory. The three types of interactions are interaction through phonons exchange, simultaneous existence of electron-phonon interaction and Coulomb interaction, and exotic pairing of electrons.

### Material and Methods:-

The attempt here is to revisit what kind of interactions can lead to a phase transition in superconductors using the theory of second quantization according to which if a perturbation commutes with the unperturbed Hamiltonian, it can lead to a phase transition.

#### Electron-phonon interaction:-

To explain the phenomena of superconductivity, large number of interactions between the electrons has been proposed. These interactions can be treated as perturbations on the unperturbed Hamiltonian (Frohlich, 1950). The first such attempt was due to Frohlich who considered the interaction between the electrons via an exchange of a phonon. The Frohlich Hamiltonian, (HF) is written as:

$$H_F = H_0 + H_{e-ph} \quad (1)$$

Where  $H_0$  is the unperturbed Hamiltonian given by

$$H_0 = \sum_k \epsilon_k C_k^+ C_k + \sum_q \hbar \omega_q a_q^+ a_q \quad (2)$$

Here the creation  $C_k^+$  and annihilation  $C_k$  operators refer to electrons and  $a_q$  refer to phonons. The value of

$H_{e-ph}$  is given by:

$$H_{e-ph} = \sum_{k,k'} m_{kk'} (a_{-q}^+ + a_q) C_k^+ C_{k'} \quad (3)$$

Where  $m_{kk'}$  is the electron-phonon matrix element, the term  $a_{-q}^+ C_k^+ C_{k'}$  refers to the scattering of an electron from  $k'$  to  $k$  with the emission of a phonon of wave vector number  $q = k' - k$  and the terms  $a_q C_k^+ C_{k'}$  refers to the scattering of an electron from  $k'$  to  $k$  with the absorption of a phonon of wave number  $q = k - k'$ . Now to understand whether the perturbation  $H_{e-ph}$  will lead to a phase transition, one has to calculate the value of  $[H_0, H_{e-ph}]$  and if it turns out to be zero, then such a perturbation can lead to a phase transition.

The purpose is to understand that if a perturbation does not commute with the unperturbed Hamiltonian, it cannot lead to a phase transition. Since Superconducting transition is a phase transition, such a perturbation cannot be considered. This method helps in the elimination of electronic interaction that cannot lead to Superconducting phase transitions.

#### Simultaneous existence of electron-phonon and Coulomb interaction:-

Another Hamiltonian also exists which is called the Nakajima Hamiltonian (Taylor, 1970) and is denoted by  $H_N$ .

In this Hamiltonian, in addition to the electron-phonon interaction, the Coulomb interaction between lattice of bare ions has been taken into account. The mutual interaction between the electrons is also added to, and is given by:

$$H_N = H_F + \sum_{k,k'} (m_{kk'}^i - m_{kk'}) (a_{-q}^+ + a_q) C_k^+ C_k + \frac{1}{2} \sum_{k,k',q} V_q C_{k'+q}^+ C_k C_k \quad (4)$$

Where is the Fourier transformation of the mutual interaction between the electrons. Now if  $H_F$  is taken as the unperturbed Hamiltonian, then the perturbation  $H_I$  will be the rest of two terms in such a system,  $H_F$  and  $H_I$  have to commute i.e.  $[H_F, H_I] = 0$ . if there is to be a phase transition.

### Exotic pairing:-

Another form of interaction between the electron in a superconductor is when the charge carriers are electrons and the pairing mechanism between the electrons is exotic (Cox and Maple, 1995). The electronic pairing in exotic superconductors is such that three electrons take part in the superconducting current and that they interact with each other through harmonic forces (Khanna and Kirui, 2002). Two of these electrons form a bound pair while the third one is a polarization electron which hops from one lattice site to another lattice site of the similar symmetry. Studies that have been done in photo-induced Raman scattering (Mihailovic et al., 1990) have confirmed that there exists strong anharmonic nature of apical oxygen vibrations. When the spectral function of electron-phonon interaction is compared with the phonon spectrum in Bismuth compounds, it is noted that both low frequency vibrations (buckling mode) and high frequency vibration (breathing mode) contribute to the electron-phonon coupling (Khanna, 2008).

It was therefore assumed that the polarization electron causes perturbation with respect to the apical oxygen vibrations leading to the contraction of  $CU_p - O_3$  bond. This perturbation is assumed to be of the form:

$$H_1 = \beta x^3 + \gamma x^4 \quad (5)$$

Where  $\beta$  and  $\gamma$  may or may not depend on the temperature. The parameter,  $x$  is given by:

$$x = \frac{1}{\alpha\sqrt{2}} (a + a^+) \quad (6)$$

Where,  $\alpha = \frac{\mu\omega}{\hbar^2}$  and  $\mu$  is the reduced mass of the pair of electrons,  $\omega$  is the phonon frequency,  $a$  and  $a^+$  are annihilation and creation operators for the electron. Now the unperturbed Hamiltonian  $H_0$  for such a system is,

$$H_0 = \frac{P^2}{2\mu} + \frac{1}{2} \mu \omega^2 x^2 \quad (7)$$

For such a system to undergo phase transition, we must have,

$$[H_0, H_1] = 0 \quad (8)$$

We will obtain the value of  $[H_0, H_{e-ph}]$  and  $[H_0, H_1]$  using theory of second quantization and see if it will lead to a phase transition.

## Result and Discussion:-

### Electron-phonon interaction:-

The Frohlich Hamiltonian,  $H_F$  forms the basis for electron-phonon interaction. We will calculate  $[H_0, H_{e-ph}]$  and if it gives a value of zero, then it can lead to a phase transition, i.e. the electron-phonon interaction can lead to a phase transition.

$$[H_0, H_{e-ph}] = (H_0 H_{e-ph} - H_{e-ph} H_0) \quad (9)$$

Replacing  $H_0$  and  $H_{e-ph}$  with the corresponding value, it gives;

$$= \left\{ \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q \right\} \left\{ \sum_{k,k'} M_{kk'} (a_{-q}^+ + a_q) c_k^+ c_k \right\} - \left\{ \sum_{k,k'} M_{kk'} (a_{-q}^+ + a_q) c_k^+ c_k \right\} \left\{ \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q \right\} \quad (10)$$

Hence electron-phonon interaction commutes and can lead to a phase transition.

**Simultaneous existence of electron-phonon interaction and coulomb interaction:-**

Nakajima Hamiltonian is denoted as  $H_N$ , in this Hamiltonian, in addition to electron-phonon interaction, the coulomb interaction between a lattices of bare ion has been taken into account. The mutual interaction between the electrons is added to  $H_N$ . thus the final form of  $H_N$  is written as;

$$H_N = H_F + \sum_{kk'} (M_{kk'}^i - M_{kk'}) (a_{-q}^+ + a_q) c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \quad (11)$$

Where  $V_q$  is the Fourier transformation of the mutual interaction between the electrons. Now  $H_F$  is taken as the unperturbed Hamiltonian, then the perturbation  $H_1$  will be the rest of two terms in such a system. Now we commute

$$H_F \text{ and } H_1$$

$$[H_F, H_1] \quad (12)$$

$$H_F = \sum_k \varepsilon_k c_k^+ c_k + \sum_q \hbar \omega_q a_q^+ a_q + \sum_{kk'} M_{kk'} (a_{-q}^+ + a_q) c_k^+ c_{k'} \quad (13)$$

And

$$H_1 = \sum_{kk'} (M_{kk'}^i - M_{kk'}) (a_{-q}^+ + a_q) c_k^+ c_{k'} + \frac{1}{2} \sum_{kk'q} V_q c_{k-q}^+ c_{k'+q}^+ c_k c_{k'} \quad (14)$$

Hence electron-phonon interaction with coulomb interaction commutes and can lead to phase transition.

**Exotic pairing of electrons:-**

In exotic pairing three electrons take part in superconducting, two of this electron forms a bond pair while the third one is a polarization electron which hops from one lattices site to another lattices site of the same symmetry. The polarization electron causes perturbation, For such a system to undergo transition; we commute perturbed and unperturbed Hamiltonian;

$$[H_0, H_1] = \left[ \left( \frac{p^2}{2\mu} + \frac{1}{2} \mu \omega^2 x^2 \right), (\beta x^3 + \gamma x^4) \right] \quad (15)$$

Hence exotic pairing commutes and can lead to a phase transition.

By considering electron-phonon interactions, simultaneous existences of electron-phonon interaction and Coulomb interaction between a lattice of bare ions and exotic pairing, and using the theory of second quantization, it was shown that such interactions leads to a phase transitions because of the commutation of perturbation. This has been shown for electron-phonon interaction, for simultaneous existences of electron-phonon interaction and Coulomb interaction and for exotic pairing.

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