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Possible Inverse Isotope effect in High Tc Superconductors Using the Non Variational Quasi-particles Formulation

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Abstract: *This theory proposes a possible isotope shift in high Tc superconductors. The attractive electron-electron pairing in the non-variational quasi-particles Hamiltonian formulation by Bogoliubov and Valatin leads due to deeply overlap of electron wave functions around* Fe^{Z+} *ion, providing an initiation for the covalent mixing of electron wave functions to form a singlet pair in the superconductivity regime. The mathematical solution yields a reversal of signs (stable and unstable energy) in the solution of the quadratic function and leads to negative isotope effect exponent.*

I. Introduction

The Bardeen, Cooper and Scheriffer (BCS)[1] bilinear model Hamiltonian (BMH) is of the form;

$$H_m = \sum_{ks} \eta_{ks} C_{ks}^{+} C_{ks} - \sum_{k} \left(\Delta_k C_{k\uparrow}^{+} C_{-k\downarrow}^{+} + \Delta_k^{+} C_{-k\downarrow} C_{k\downarrow} - \Delta_k b_k^{+} \right) \quad 1$$

$$H = \quad - \sum_{1} V_{k1} \left(C_{-k\downarrow} C_{k\downarrow} \right) = - \sum_{1} V_{k1} \left(b_1 \right) \quad 2$$

Since this form of mean field Hamiltonian is bilinear in the creation and annihilation operators. We diagonalized by using a linear canonical transformation of these operators introduced by Bogoliubov and Valatin (BV)[2-4].

$$C_{k\downarrow} = U_k \gamma_{ko} + V_k^{+} \gamma_{k1}^{+} \quad , \quad C_{-k\downarrow}^{+} = -V_k \gamma_{ko} + U_k^{+} \gamma_{k1}^{+} \quad 3$$

γ_{ko} , γ_{k1} are fermions annihilation operators,the coefficient U_k , V_k are chosen to make the Hamiltonian diagonal and also for the coefficients of $\gamma_{k0}^{+} \gamma_{k1}^{+}$ and $\gamma_{k1} \gamma_{k0}$ in the MH to vanish and are required to satisfy

$$U_k^2 + V_k^2 - 2U_k V_k + 2V_k U_k = 1 \quad 4$$

Putting Eqn(3) into Eqn(1), upon simplification, we obtain

$$H_m = \sum_{ks} \eta_{ks} \left[\left(U_k \gamma_{ko} + V_k^{+} \gamma_{k1}^{+} \right) \left(-V_k \gamma_{ko} + U_k^{+} \gamma_{k1}^{+} \right) \right] - \sum_{k} \left(\Delta_k \left[\left(-V_k \gamma_{ko} + U_k^{+} \gamma_{k1}^{+} \right) \left(U_k \gamma_{ko} + V_k^{+} \gamma_{k1}^{+} \right) \right] \right)$$

$$\sum_{k} \Delta_k^{+} \left[\left(\left(U_k \gamma_{ko} + V_k^{+} \gamma_{k1}^{+} \right) \left(-V_k \gamma_{ko} + U_k^{+} \gamma_{k1}^{+} \right) \right) \right] - \sum_{k} \Delta_k b_k^{+} \quad 5$$

The Hamiltonian is diagonalized if we select U_k and V_k so that the co-efficient of $\gamma_{k0}^{+} \gamma_{k1}^{+}$ and $\gamma_{k1} \gamma_{k0}$ vanish. This means that the Hamiltonian is carried into a pair containing only constant plus terms proportional to the occupation number $\gamma_{ko} \gamma_{k1}^{+}$. The coefficient of undesired terms is zero, than get

$$0 = \sum_{ks} \eta_{ks} \left[2 |V_k|^2 \right] + \sum_{k} \left(\Delta_k U_k V_k^{+} + \Delta_k^{+} U_k^{+} V_K^{+} (-1) \right) \quad 7$$

Multiplying both sides by $U_k V_k$, and applying $\sum_k \to \int dk,\ \int U_k^+ U_k dk = \int V_k^+ V_k dk = \int |V_k|^2 dk = 1$

Upon multiplication with $\frac{\Delta_k^+}{U_k^2}$, rearranging and simplification yields a quadratic function of the form;

$$\left(\frac{V_k}{U_k}\right)^2 \Delta_k + 2\eta_k \left(\frac{V_k}{U_k}\right) - \Delta_k = 0 \qquad 8$$

Resolving Eqn (8) by completing the square method,

$$\left(\frac{V_k}{U_k}\right)^2 + \frac{2\eta_k}{\Delta_k}\left(\frac{V_k}{U_k}\right) = \frac{\Delta_k}{\Delta_k} \qquad 9$$

$$\left(\frac{V_k}{U_k} + \frac{2\eta_k}{2\Delta_k}\right)^2 = \frac{\Delta_k^2 + \eta_k^2}{\Delta_k^2} \qquad 10$$

$$\frac{V_k}{U_k} = \frac{\eta_k}{\Delta_k} + \frac{\sqrt{\Delta_k^2 + \eta_k^2}}{\Delta_k^2},\ \frac{V_k}{U_k} = \frac{\eta_k}{\Delta_k} - \frac{\sqrt{\Delta_k^2 + \eta_k^2}}{\Delta_k^2} \qquad 11$$

Observing the math's solutions[4-6] reveals the existence reversal of signs in Δ_k and E_k arise naturally from the method of solution of the quadratic function resulting to the stable and the unstable solutions of the energy

$$\left(\frac{V_k}{U_k}\right)\Delta_k = -\eta_k - \left(\eta_k^2 + \Delta_k^2\right)^2,\ E_k = \left(\eta_k^2 + \Delta_k^2\right)^2 \qquad 12$$

The negative sign is chosen in other to constructively criticized, challenged the statement that the positive sign corresponds to the stable state solution of energy and not the negative. E_k, gives the energy of excitation, Δ_k plays the role of an energy gap or minimum(maximum) energy excitation since at the Fermi level where $\eta_k = 0,$ $E_k = |\Delta_k\rangle 0.$ Applying $V_k U_k = \frac{\Delta_k}{2E_k}$, $U_k^2 = 1 - V_k^2$, $\frac{V_k}{U_k} = \frac{-E_k - \eta_k}{\Delta_k}$, $\frac{U_k}{V_k} = \frac{\Delta_k}{-E_k - \eta_k}$ to get the unstable square solution in V_k , U_k and the equivalent solution in BCS we obtain

$$U_k^2 = 1 - \frac{\Delta_k}{2E_k} \bullet \frac{V_k}{U_k} = 1 - \frac{\Delta_k}{2E_k} \bullet \frac{-E_k - \eta_k}{\Delta_k} = 1 - \frac{\Delta_k}{2E_k}\left(\frac{-E_k}{\Delta_k} - \frac{\eta_k}{\Delta_k}\right) \qquad 15$$

$$U_k^2 = \left(1 + \frac{1}{2} + \frac{\eta_k}{2E_k}\right) = \left(\frac{3}{2} - \frac{\eta_k}{2E_k}\right),\ U_k^2 = \frac{1}{2}\left(3 + \frac{\eta_k}{E_k}\right),\ V_k^2 = \frac{1}{2}\left(3 - \frac{\eta_k}{E_k}\right) \qquad 16$$

While Eqn (15) and Eqn (16) differ slightly with the result of BSC in signs and in number, It is also greater than the stable solution of Eqn (17) (which agrees very well with BCS) by the factor 3.

$$U_k^2 = \frac{1}{2}\left(1 - \frac{\eta_k}{E_k}\right),\ V_k^2 = \frac{1}{2}\left(1 + \frac{\eta_k}{E_k}\right) \qquad 17$$

The diagonalized model Hamiltonian becomes

$$H_m = -\sum_k \left(\eta_k - E_k + \Delta_k^+ b_k^+\right) - \sum_k E_k \left(\gamma_{k0}^+ \gamma_{k0} + \gamma_{k1}^+ \gamma_{k1}\right) \qquad 18$$

The first sum in the equation of the band is constant which differ from the corresponding sum for the normal state. T = 0, $\varepsilon_k = |\eta_k|$, $\Delta_k = 0$ by exactly the condensation energy $U_s(0) - U_n(0) = \frac{1}{2}N(0)\Delta(0)$, U(T) = internal energy, $\Delta_k = 0$ is the energy gap at T=0. The second sum gives the increase in energy above the ground state in terms of the number operators for Fermions. $b_k = \langle C_{-k\downarrow} C_{k\downarrow} \rangle$ applying the values of $C_{-k\downarrow} C_{k\downarrow}$ into the equation and dropping off-diagonal terms in quasi-particle operator. Equation emphasizes the rudiment of the superconductivity model for the superconducting iron oxy-pnictide materials, attractive electron-electron pairing due to deep overlapping of electron wave functions around Fe^{Z+} ion of effective valence (Z), provides an initiation for the covalent mixing of electron wave functions to form a singlet pair, $C_{-k\downarrow} C_{k\downarrow}$ HM[7-9].

$$b_k = \langle C_{-k\downarrow} C_{k\downarrow} \rangle = U_k V_k \langle 1 - \gamma_{k0}^{+} \gamma_{k0} + \gamma_{k1}^{+} \gamma_{k1} \rangle \qquad 19$$

While the energy gap expressions are

$$\Delta_{1k} = \sum_{1k} V_{k1} b_{k1} = \sum_{1k} V_{k1} \langle C_{-1k\downarrow} C_{1k\downarrow} \rangle = \sum_{1k} V_{k1} U_k^{+} V_k^{+} \langle 1 - \gamma_{k0}^{+} \gamma_{k0} + \gamma_{k1}^{+} \gamma_{k1} \rangle \qquad 20$$

At T= 0, equations reduces to Eqn (1) but at T > 0, the probability of a fermions quasi-particle with excitation energy, E_k is the Fermi- Dirac distribution, $F(E_k) = \exp(\beta\varepsilon_k + 1)^{-1}$

$$\Delta_k = \sum_{1k} V_{k1} \frac{\Delta_1}{2E_1} (1 - 2F(E_k)) \qquad 21$$

Δ_k , being temperature dependent, the integral equation has a trivial solution for $\Delta_k = 0$ which corresponds to the normal state (NS). Non trivial solution exists if the NS is unstable and the system becomes superconducting. The equation above gives the superconducting state as long as the gap parameter for Δ is non-zero.

$\Delta_k = \Delta_k^1 = \Delta, \mathrm{E}_k = \eta$, approaching this equation Coopers way[10]

$$V_{kk^1} = \begin{cases} -V, |\eta_k|, |\eta_{k^1}| < \hbar\omega \\ 0, \ otherwise \end{cases} \qquad 22$$

Where $-V = \langle V_{ph} \rangle + \alpha \langle V_s \rangle$, α is constant less than unity. For weak superconductors, N(0)V << 1 and N(0)V >> 1 for strong coupling superconductors. Changing the sum over k to the density of states $N(\eta_k)$

$$1 = -V \sum_{k, \eta_k | < \hbar\omega} \frac{\tanh(\eta_k / 2K_\beta T_c)}{2\eta_k} = -V \int_{\hbar\omega_D}^{\hbar\omega_D} N(\eta_k) \frac{\tanh(\eta_k / 2K_\beta T_c)}{2\eta_k} \qquad 23$$

ω_D , is Debye cut-off frequency such that[11] $\hbar\omega_D = K_\beta \theta_D$. Since the density of state in the NS varies little within an energy $\hbar\omega_D$ of the Fermi level and also $N(\eta_k)$ can be approximated by the constant value N(0) at the Fermi level

$$1 = -VN(0) \int_0^{\hbar\omega_D} \frac{d\eta}{\eta} \frac{2\tanh(\eta_k / 2K_\beta T_c)}{2} \qquad 24$$

Upon simplification of Eqn(24), we obtain the gap equation, critical temperature and apply it to weak coupling limits.

$$-T_c = 1.13\theta_D \exp(-\lambda_{eff}) \ , \ \frac{\Delta(T)}{K_\beta T_c} = 2\exp\left(\frac{-13.6}{Z}\right) \qquad 25$$

Since isotope effect exponent is as a results of the discovery of the interaction of electron-electron in the self consistence phonon mediated superconductivity. Hence, it value for iron pnictides can be got from the transition

temperature or the gap equations. Using this relation [12], $w_\beta = \left(\frac{K_\beta}{m}\right)^{\frac{1}{2}}$ and solving with Eqn(25), we obtain that

$$-T_c = 1.13m^{-\frac{1}{2}}\left(\hbar(\mathrm{K}_\beta)^{-\frac{1}{2}}\right)\exp\left(-\lambda_{eff}\right) = cm^{-\frac{1}{2}} \qquad 26$$

Therefore, $C = \left(1.13\hbar(\mathrm{K}_\beta)^{-\frac{1}{2}}\exp\left(-\lambda_{eff}\right)\right)$

Energy gap, transition temperature and isotope effect exponent can be predicted in the iron based superconducting materials from Eqn(25) and Eqn(26).Thus, isotope effect exponent is BCS and negative (-0.2).

II. Summary and Conclusion

This theory shows that mathematical calculations of energy gap, transition temperature, isotope effect exponent and assumes from mathematical deductions that coherent length, penetration depth, specific heat and other properties have negative values. These contradict experimental and theoretical findings. However, It remains valid for property, such as isotope effect exponent and in agreement with theories and experimental predictions of isotope shift in iron pnictides and cuprates.

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