

Ground State Energy of Induced Superconductivity and Its Variation with Inter- Atomic Distance

Alphayo A. O¹, Barasa H. W¹, Rapando W. B¹.

¹Masinde Muliro University of Science and Technology, P.O Box 190-50100, Kakamega, Kenya.

Abstract- We subject the superconducting order parameter of induced superconductivity derived in the proximity effect to Schrodinger Equation in order to calculate ground state to Schrodinger Equation in order to calculate ground state energy of the induced superconductor. Both superconducting cuprates (such as Hg1223, Tl1220, LnFeASO_{0.6}) and pure metals (such as Lead, europium and iron) are used as the neighboring materials to the superconductor. Among the superconducting mater which has the shortest inter-atomic distance ials, the Hg1223 highest energy is found in LnFeASO_{0.6} while) with the longest inter-atomic distance showed the lowest energy of the system. For pure metals the highest energy of the system was found in lead metal with the longest inter-atomic distance while) the lowest energy of the system was found to be in iron metal with the shortest inter- atomic distance. This knowledge is important as it can be applied in Josephson's junctions and SQUIDS.

Keywords: Ground State Energy, Induced Superconductivity, Inter-Atomic Distance.

1. INTRODUCTION:

Energy of pairing interaction in superconductors is known to be weak; of the order 10^{-3} eV. This makes it easy for the thermal energy to break the pairs. This is why at low temperatures in metals and other substances, a good number of electron cooper pairs exist but few, at high temperatures (Zheng and Chan 2016). Thus, knowledge of ground state energy is vital in predicting whether or not, pairing would take place. The Superconducting state is characterized by some energy scales. These are energy gap, coherence gap, phase stiffness and condensation energy. The pairing energy gap measures the strength of the binding of electrons into the cooper pairs. This means that the value of the binding energy between the electrons corresponds to energy gap. The electron pairing energy depends on temperature (Odhiambo, Sakwa, Ayodo & Rapando, 2016). Both electron pairing and long range phase coherence which are independent from each other are required by a superconductor. They both happen at different temperatures, that is temperature at which long range coherence occur was identified to be lower than that at which pairing of electrons take place. Hainze & Seiringer, (2013) however found out that in conventional superconductors the temperatures at which both pairing of electrons and long range coherence occur are similar. The magnitude of phase stiffness influences the simultaneous happening of electron pairing and long range phase coherence occurring.

The energy gap depends on the thickness of the normal metal and the distance of the interface between the metals and the superconductor (Rainer, 2016). The phase coherence is mediated by the overlap wave functions of the electron pairs in conventional superconductors. This process does not lead to a new order parameter but enlarges the wave functions of the pairs of electrons to an order parameter level (Heikkinen, Kim, Troyer and Torma, 2014). This means that the electron pairing and phase coherence simultaneously take place at similar temperatures. The phase coherence energy gap, becomes the Cooper pairs condensation energy the moment the long range phase coherence emerges. Since phase stiffness has a significance influence on the simultaneous occurrences of electron pairs, on the other hand binding energy between the electrons corresponds to energy gap and entire energy of the system.

It has been established that in good high temperature superconductors, $T_c \sim 300K$, the rate of change of the energy of the system at high temperatures must be as low as possible. (Rapando *et al*, 2015). In this research, we endeavor to establish whether this can be obtained through variation of inter-atomic distance in the induced superconductor.

2. THEORETICAL FORMULATION:

We assume a good contact between a superconductor crystal and another crystal at ambient temperature. In our previous work, (Ocholla *et. al*, 2017) we obtained the wave function of induced superconductivity in the proximity effect

$$\psi(x) = -\frac{Q\pi^2}{4a^2n_3} \cos(nx)$$

$$\text{Where } Q = \frac{2n \dots^* \cdot 2 \cdot 2}{AK_B \hbar^2 (ab)^2}$$

as; a is inter-atomic spacing, n is Fourier integer variable, k is wave vector, λ is wavelength, V is linear velocity, h is plank constant, \hbar is the phase stiffness, m^* is the effective mass of charge carrier, A is the dimensionless number of order 1 which depends on the details of short distance physics, b is extrapolation distance and K_B is Boltzmann Constant.

According to quantum mechanics, any measurable value expected to be observed in the superconducting state can be obtained by expression (Andrei, 2004)

(Quantum Operator) (Measured Value)

The quantum operator corresponds to a measurable quantity. This means that the measured value is the eigen value corresponding to Eigen function.

We subject the wave function of induced superconductor to the Schrodinger equation in order to calculate the ground state energy of the system. The three dimensional Schrodinger equation is sited as (Anderson, 2009)

$$H(r) \psi(r) = E \psi(r) \dots \dots \dots (2)$$

Where H is Hamiltonian operator, $V = \frac{1}{2}kr^2$ is

scattering potential and E is ground state energy For simplicity a one dimensional case where $r=x$ is considered. The Hamiltonian operator then

becomes $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$ and Scattering potential $V(x) = \frac{1}{2}kx^2$

Then eqn. (2) becomes:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \left(\frac{Q\pi^2}{4an} \right) = E \left(\frac{Q\pi^2}{4an} \right) \dots \dots \dots (3)$$

Eqn. 3 reduces to,

$$-\frac{Q\pi^2}{8ma^2n} = \frac{1}{2} \left(\frac{Q\pi^2}{4an} \right) E \dots \dots \dots (4)$$

Which can quite easily be simplified to,

becomes $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$ and Scattering potential $V(x) = \frac{1}{2}kx^2$

Then eqn. (2) becomes:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \left(\frac{Q\pi^2}{4an} \right) = E \left(\frac{Q\pi^2}{4an} \right) \dots \dots \dots (3)$$

Eqn. 3 reduces to,

$$-\frac{Q\pi^2}{8ma^2n} = \frac{1}{2} \left(\frac{Q\pi^2}{4an} \right) E \dots \dots \dots (4)$$

Which can quite easily be simplified to,

becomes $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$ and Scattering potential $V(x) = \frac{1}{2}kx^2$

Then eqn. (2) becomes:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \left(\frac{Q\pi^2}{4an} \right) = E \left(\frac{Q\pi^2}{4an} \right) \dots \dots \dots (3)$$

Eqn. 3 reduces to,

$$-\frac{Q\pi^2}{8ma^2n} = \frac{1}{2} \left(\frac{Q\pi^2}{4an} \right) E \dots \dots \dots (4)$$

Which can quite easily be simplified to,

$$\left(\frac{Q\pi^2}{8a^2n} \right) \left(\frac{2}{m} \frac{kx^2}{n} \right) = \frac{EQ\pi^2}{4an} \cos(\pi x) \dots \dots \dots (5)$$

$\frac{4a^2n}{Q\pi\epsilon_0}$

When both sides of equation (5) are multiplied by $\frac{4a^2n}{Q\pi\epsilon_0}$ we obtain,

$$\frac{-\frac{1}{2} \left(\frac{2n^2}{m} + \frac{kx^2}{2} \right)}{2 \left(\frac{2n^2}{m} + \frac{kx^2}{2} \right)} \dots \dots \dots$$

Rearranging equation (6), equation (7) is obtained.

$$E = \frac{1}{2} \left(\frac{2n^2}{m} + \frac{kx^2}{2} \right) \dots \dots \dots (7)$$

Equation (7) gives the ground state energy of the induced superconductor.

For superconductivity to take place, low energy of the system is required therefore, pure metals with shorter inter-atomic distances can be used to make superconductors through proximity effect because they tend to maintain low energy of the system as the cooper pairs move into the metal.

To break chemical bonds between the cooper pairs, a minimum amount of energy is required. The energy gap represents the energy required to break these electron pairs. Electrons which take up states near and even Fermi energy can easily move into the empty states. At the S-N junction, the ion thermal vibration at N has almost a similar frequency to that in the S-system. Thermal vibration of lattice ions in N are higher since the n-crystal is at room temperature. This leads to exponential growth in energy, a condition that causes the breaking of cooper pairs. Thus, superconductivity disappears as we move deeper into the N- Crystal.

Likewise, when the temperature is high, the electrons at state below the energy gap gain more kinetic energy and tend to move across the gap while the state above the gap become filled with single electrons, this makes it easier for electrons to scatter off making the material to lose its superconducting state (Saxena, 2012). Energy in the scattering process enables electrons to get into unoccupied state, electrons then change their states, dissipation occurs and hence there is electrical resistance (Annics et. al, 2008). The energy gap reduces gradually as the temperature increases above Tc; having known that the energy gap determines the electron binding energy, small gap would mean low electron binding energy.

3. RESULTS AND ANALYSIS

3.1 GROUND STATE ENERGY OF INDUCED PURE METAL SUPERCONDUCTORS

Using equation (7), the plot of figure 1.1 was obtained.

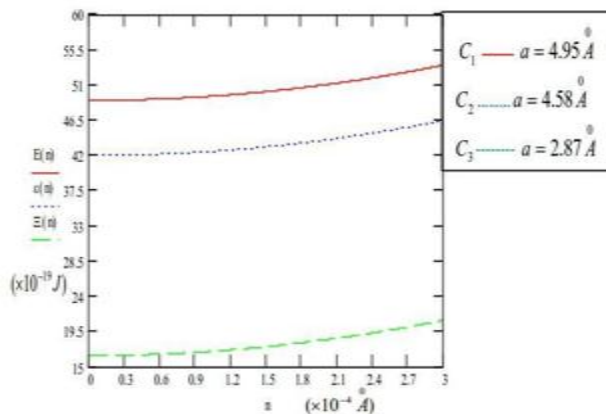


Figure 1.1: Variation of Ground State Energy of induced superconductivity and Inter-atomic distance of Pe , Eu and fe

Here inter-atomic distances of 4.95A, 4.58 A and .87A obtained from lead, europium and iron metal . respectively were used to plot the graph. From figure 1.1, the plotted result displayed exponential growth of the energy of the system for an induced superconductor as the cooper pairs penetrate into the pure metals. The trend revealed a relationship with both inter-atomic distance and Fourier integer as the electron pairs move deeper into the pure metals.

At the S-N boundary iron metal, europium metal and iron metal showed energy of $16.5 \times 10^{-19} J$, $43.0 \times 10^{-19} J$ and $48.7 \times 10^{-19} J$ in that order. The highest energy of the system was found in lead metal with the longest inter-atomic distance while the lowest energy of the system was found to be in iron metal with the shortest inter-atomic distance.

5.2. GROUND STATE ENERGY OF SUPERCONDUCTIVITY INDUCED INTO THE SUPERCONDUCTING MATERIALS

Using equation (7) the plot of figure 1.2 was obtained.

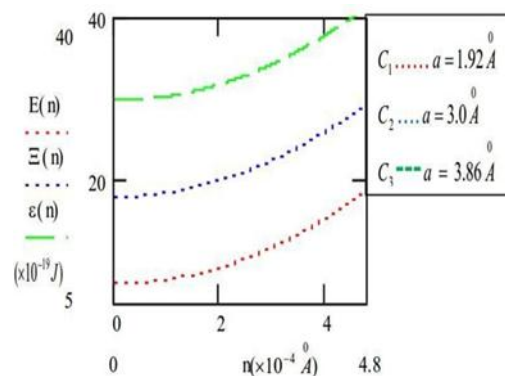


Figure 1.2: Variation of ground state Energy of induced superconductivity and Inter-atomic distance The plotted result exhibited upward growth of the energy of an induced superconductor as it progresses into the neighboring superconducting material, assumed to be at room

temperature. A trend was identified that revealed a relationship with inter-atomic distance and Fourier integer respectively after distortion, resulting in exponential growth of energy as the cooper pairs penetrate into S2.

Curve C₁ represents mercury cuprates with a ≈ 1.92 Å. Are corded lowest energy of the system among the three cuprates. Its energy at the S-S boundary was 7.2×10^{-19} J then grew exponentially. At the junction, energy of the system in Thallium based cuprate represented by C₂ having a ≈ 3.0 Å was noted to begin from 18.6×10^{-19} J also maintained the trend of exponential growth as the cooper pairs penetrate deeper into S2. Iron based superconducting material at a ≈ 3.86 Å had the highest energy of the system beginning at 30.3×10^{-19} J and grew exponentially as the cooper pairs move into the superconductor.

These results reveal that to maintain low energy and hence keep induced superconductivity, inter-atomic distance of the crystal into which superconductivity is being induced must be as small as possible. Such systems of low energy e.g Hg1223 also attain high transition temperatures. In these systems, electron transfer energy t , is maximized (Rapando, et al, 2016), leading to d- wave pairing.

Heinze *et. al*, (2013) found out that when two or more sets of strong interactions are closer to each other, they can lower their energy by sharing the same distortions, which leads to an effective attraction between them. This mechanism basically lowers the energy of the system in superconducting materials where as in pure metals there is delocalization of electrons leading to coulomb repulsion among the existing single electrons, when the coulomb repulsion forces are quite high, energy of the system rises.

The variation of energy with inter-atomic distance in superconducting materials revealed in this research agrees with Kamashev *et. al*, (2017), who observed that with increasing inter atomic distance, the energy the Pb/Cu bilayers shows an increase in energy of the system. Lattice impurities and other defects in the material prevent the material from becoming a perfect superconductor (Orphur, 2015). Mercury based cuprates showed lowest system energy which is good for electron pairs; at low energies of the system the electron scattering will not be experienced. To make a better superconductor through proximity effect, an individual requires materials which can maintain low energies to prevent pairing electron scattering.

6.CONCLUSION:

We have ascertained that the energy of the induced superconductor is lowest at the boundary but increases exponentially with increase in distance as one move into the induced superconductor. Crystals with shorter inter-atomic

distances exhibit low ground state energy, a prerequisite condition for high temperature superconductivity. Through proximity effect, we can obtain superconductors at room temperature as long as the contact between the two crystals is good enough. Pure metals may not make good superconductors by this method compared to Cuprates given the high ground state energy they exhibit.

ACKNOWLEDGEMENT:

We sincerely appreciate Masinde Muliro University of Science and Technology for the Conducive research environment they accorded us in the process of carrying out this research.

REFERENCE:

- [1] Anderson, P. "Condensed Matter physics". *Journals for Superconductivity and Magnetism*, 2009. Vol. 19, pp. 13- 17.
- [2] Andrei M. "Room Temperature Superconductivity", Great Abington, *Cambridge International Publishers*, 2004, pp 40-60 UK.
- [3] Annica, M., Schaffer, B. & Doniach, S. "Self-Consistent Solution for Proximity Effect and Josephson Current in Ballistic Graphene SNS Josephson Junctions". 2008. *Phys Rev. B* 78 pp 354-443
- [4] Hainze, G., & Seiringer, R. "Critical Temperature and Energy Gap for the BCS Equation". *Journals for Superconductivity and Magnetism*, 2013. Vol. 14, pp. 10, 35.
- [5] Heikkinen M. O. J., Kim D.-H., Troyer M., & Torma P., "Nonlocal Quantum Fluctuations and Fermionic Superfluidity in the Imbalanced Attractive Hubbard Model," 2014. *Physical Review Letter*. 14 (2) Pp 113, 185301.
- [6] Kamashev A.A., Leksin P.V., Schumann J., Kataev V., Thomas J., Gemming T., Büchner B., & Garifullin I.A., "Proximity effect between a superconductor and a partially spin-polarized ferromagnet: Case study of the Pb/Cu/Co₂Cr_{1-x}FexAl trilayer" *Phys. Canadian Journal of Physics*. 2017, 7(3) pp 677-842.
- [7] Ocholla A., A., Rapando W., B., Barasa H., W. & Ayodo K., Y. "Wave Function of Induced Superconductivity: Proximity Effect". *International Journal of Multidisciplinary Science and Technology*. 2017, Vol. 02 (10) pp 10-19.
- [8] Odhiambo J. O., Sakwa T. W., Rapando B. W. & Ayodo Y. K. "Effect of CuO₂ Plane on the Thermodynamic Properties of Double Tl-O Layered Cuprate Based on an Interaction between Cooper Pair and an Electron". *International Journal of Physics and Mathematical Sciences*. 2016, Vol 3 (2), pp 227-251.

- [9] Orphur, F. "An Existence Theorem for the BCS integral Equation". *Journal of Research and Development*, 2015. Vol. 8(4) pp 187-188.
- [10] Rainer K. "SQUIDS in biomagnetism: a roadmap towards improved healthcare". *Superconductor Science and Technology Journal*. 2016, Vol. 29(9), pp 34-56
- [11] Rapando B.W, Khanna K. M, Tonui J.K, Sakwa T. W, Muguro K. M, Kibe H, Ayodo Y.K, Sarai A. "The Dipole mediated t-J Model for High-Tc Superconductivity". *International journal of Physics and Mathematical Sciences*, Vol. 5(3), Sep. 2015, pp 32-37.
- [12] Rapando B. W, Tonui J.K, Khanna K.M, Mang'are P.A. "The Diagonalized t-J Hamiltonian and the thermodynamic properties of High - Tc Superconductors". *American Research Journal of Physics*, Vol. 2016, pp1- 11.
- [13] Saxena A. K. "High Temperature Superconductors". Springer Series in Material Science. Springer-Verlag Berlin. 2012
- [14] Zheng B.-X. & Chan G. K.-L. "Ground-state phase diagram of the square lattice Hubbard model from density matrix embedding theory," *Physical Review*, 2016. B 93, (13) 351-426.

BIOGRAPHY:

Third author; Dr. Rapando Wakhu; Lecturer, Dpt. of Physics, Masinde Muliro University of Science and Technology

