Phase Transition in High Temperature Superconductivity

[1*]KANDIE, D. K., [2]M. K. KHANNA., [2]P.C. KORIR and [2]S.C. LIMO

[1]Department of Physics, Laikipia University, Nyahururu, Kenya

[2]Department of Physics, University of Eldoret, Kenya

Corresponding Author E-mail addresses: kiplangatkandie@yahoo.com

Abstract

The onset of superconductivity is accompanied by abrupt changes in various thermodynamic properties, which is the hallmark of a phase transition. At the superconducting transition, it suffers a discontinuous jump and, therefore, ceases to be linear resulting in change of volume, specific heat and entropy at the critical temperature T_C. Phase transitions are of first order when the latent heat $L = 0$, and are of the second-order phase transition when there is a specific heat jump at the transition temperature T_C. In this study the variation of specific heat capacity with temperature for high temperature superconductors changes discontinuously but does not become infinite at T_C showing a finite specific heat jump at the transition temperature and hence the phase transition is of second order.

Keywords: Phase Transition, Superconductivity, Critical Temperature

Introduction

The vanishing of electrical resistance of a conductor at very low temperature is known as the phenomena of superconductivity. It was discovered by H. K, Onnes in 1911 at Laiden, Holland [1]. He found that when the temperature of pure frozen mercury was reduced below 4.2K, its electrical resistance disappeared resulting in the flow of large electrical currents. A great number of pure metals, alloys and doped semiconductors were found to have this property. It is also found that the metals cooled in the superconducting state in a moderate magnetic field expel the magnetic field from its interior resulting in negative susceptibility of the material and this is the property of a diamagnetic material. Thus a superconductor is a diamagnetic and this is called Meissner effect that was discovered in 1933 by Meissner *et al* [2, 3].

The discovery of high T_C Cuprates and their peculiar properties has stimulated enormous theoretical interest to search for the origin of pairing mechanism in these systems and also to decide whether the superconducting transition is a first-order or second-order phase transition. Superconductors and superfluids exhibit phase transitions [4]. Superconductivity results from correlations between motions of electrons in a metal, induced by electron-phonon interactions.

Its study has been important for our understanding of these interactions and has produced great insight into the physics of electrons in metals at low temperatures.

Since superconducting current is carried by electrons, there will be Coulomb repulsion within them. The Coulomb repulsion could be sometimes very large and or sometimes less than some critical value (V_C); it is found that in the first case, transition to super-conducting state is of first-order and in the second case it is of second-order. In this study the problem focus is to study the order of phase transition in high T_C superconductors [5]. The order of phase transition is determined by knowing whether the latent heat is finite (first-order phase transition) or there is a jump in the specific heat (second-order phase transition)

Theory

In thermodynamics, phase transition is the transformation of a thermodynamic system from one phase to another. The distinguishing characteristic of a phase transition is an abrupt sudden change in one or more physical properties, in particular the heat capacity, with a small change in thermodynamic variables such as the temperature.

The first-order phase transition involves a latent heat. During such transition a system either absorbs or releases a fixed amount of heat [6]. Because energy cannot be instantaneously transferred between the system and its environment, first-order transitions are associated with “mixed-phase regimes” in which some parts of the system have completed the transition and others have not.

The second class of phase transition is the “continuous phase transition”, also called second-order phase transitions and not associated with latent heat. Examples of second-order phase transition are the ferromagnetic transition and the Superfluid transition [7, 8].

In superconducting materials, the characteristic of superconductivity appear when the temperature T is lowered below a critical temperature T_C . The value of this critical temperature varies from one material to the other. Conventional superconductors usually have critical temperatures ranging from 1K to 20K. Cuprate superconductors can have much higher critical temperatures. $YBa_2Cu_3O_7$, one of the first Cuprate superconductors to be discovered, has a critical temperature of 92K, and mercury Cuprates have been found with critical temperatures in excess of 130K[8]. The explanation for these high critical temperatures remains unknown. Electron pairing due to phonon exchanges explains superconductivity in conventional superconductors, but it does not explain superconductivity in the newer superconductors that have a very high T_C

Methodology

Condensation into a superconducting state lowers the free energy F_n of the normal state to F_s of the superconducting state. The critical field H is given by the relation [9].

$$\frac{H_C^2}{2\mu_0} = F_n - F_s \qquad \text{.......................} (1)$$

The specific heat constant γ is given by

$$\gamma = \frac{1}{3}\pi^2 D(\varepsilon_F) K_B^2 \qquad \text{.......................} (2)$$

From the BCS theory [3, 6] based on equations (1) and (2) we have the relation,

$$H_C(0) = \left(\frac{3\mu_0}{2}\right)^{\frac{1}{2}} \cdot \frac{3.5}{2\pi} \gamma^{\frac{1}{2}} T_C = 7.65\times10^{-4}\gamma^{\frac{1}{2}} T_C \qquad \text{.......................} (3)$$

Thermodynamic description of a superconductor

Although the Meissner effect is described quite accurately by linear relation between the intensity of the magnetization M and the magnetic field H, this linearity does not persist with the arbitrarily high magnetic fields. The most striking non-linear effect is the existence of a critical magnetic field for superconductivity. For instance, for a small value of magnetic field, H_0 a superconductor may exhibit Meissner effect but at some critical field strength H_C, the situation may change abruptly; the specimen losses the property of superconductivity, there is a thermodynamic transition back to the normal state, with a latent heat of transition.

According to Ehrenfest such a transition is called first order phase transition, at constant temperature and constant applied magnetic field, heat must be supplied to the specimen to enable it to make the transition from the superconducting to the normal state. However, when there is no acting external magnetic field $H_C(T_C) = 0$ and the temperature $T \to T_C$ (the critical temperature for superconducting transition), the latent heat is zero. Such a transition is called the second order phase transition. The electronic specific heat jumps discontinuous to about three times the normal value γT_C as we cool through the transition (γ is a constant value) temperature T_C.

We now have to calculate the jump in the specific heat as the material undergoes transition from the normal to the superconducting state. The change in the Gibb's Free energy density of a system, when the external magnetic field is changed has to be written.

Thus we write;

$$dG = -SdT - \frac{1}{4\pi} B.dH \text{ ....} (4)$$

where S is the entropy per unit volume.

Equation (6) gives

$$S_s = -\left(\frac{\partial G}{\partial T}\right)_H \quad \text{and} \quad B = -4\pi\left(\frac{\partial G}{\partial H}\right)_T \text{ ....} (5)$$

Specific heat C_H is now given as

$$C_{HS} = -T\left(\frac{\partial S}{\partial T}\right)_H \text{ ....} (6)$$

Considering a long superconducting cylinder in a magnetic field that is parallel to the axis of the cylinder, that is $H = H_Z$, and then increase the value of H from zero to some value H we have at constant temperature T,

$$G_S(T,H) - G_n(T,H) = \frac{1}{8\pi}\left[\{Hc(T)\}^2 - H^2\right] \qquad (7)$$

The entropy S is given by

$$S_s(T,H) - S_n(T,H) = -\frac{1}{4\pi} H_C(T)\frac{dH_C(T)}{dT} \qquad (8)$$

And the latent heat Q_L is,

$$Q_L = T(S_s - S_n) = -\frac{1}{4\pi} TH_C(T)\frac{dH_C(T)}{dT} \qquad (9)$$

The empirical relation for the variation of $H_C(T)$ with the temperature T is

$$H_C(T) = H_C(0)\left[1 - \left(\frac{T}{T_C}\right)^2\right] \qquad (10)$$

The Specific heat based on equation (6) is given as,

$$C_{Hs} - C_{Hn} = \frac{T}{4\pi}\left[\left(\frac{dH_C}{dT}\right)^2 \pm H_C\frac{d^2H_C}{dT^2}\right] \qquad (11)$$

The jump in the specific heat at $T = T_C$ is given by,

$$\left(C_{HS} - C_{Hn}\right) = (\Delta C)_{T=T_C} = \frac{T_C}{4\pi}\left[\left(\frac{dH}{dT}\right)_{T=T_C}\right]^2 \qquad (12)$$

Equation (12) is the Rutgers Formula.

First-Order Phase Transition.

In a phase change the change involves a major re-arrangement of structure of the substance, resulting in change of volume, specific heat, entropy viscosity etc at the critical temperature T_C .

Since such changes involve energy, energy change, input or output produced at a finite amount of heat, the latent heat L, the transition takes place at a constant temperature T of ΔT or dT = 0. When a substance undergoes a change of phase from phase 1 to phase 2, the accompanied latent heat is

$L_{12} = T_c(S_2 - S_1)$.. (13)

where S_1 is the entropy in phase 1 and S_2 is the entropy in phase 2. Then this equation shows that there is a discontinuity in entropy since the heat capacity C_P is,

$$C_P = T\left(\frac{\partial S}{\partial T}\right)_P \quad \text{.. ....} \quad (14)$$

Second-Order Phase Transition.

There are other changes of phase involving the initiation of a different kind of ordering in a crystal lattice or the appearance of Superfluid in Helium II, or super-fluidity of a nuclear system and the appearance of the solid and a super-solid ^{4}He, and also superconductivity of such phase changes may involve a change of slope of S against T at the transition point, not a change of the value. In this case the heat capacity changes discontinuously but does not become infinite at T_C. Such changes are called phase change of the order. For such changes, there is no discontinuity in volume ($V_1 = V_2$) and or entropy ($S_1 = S_2$) during the transition.

Phase Transition in Superconductors

Phase transitions are of first-order when the latent heat $L = 0$, and are of the second-order phase transition when there is a specific heat jump at the transition temperature T_C (2.17K in ^{4}He liquid)

A recent study has opened up the possibility of investigating the crossover from a Bose-Einstein Condensate (BEC) to a Bardeen-Cooper-Schrieffer (BCS) Superfluid [9]. In these systems the strength of the interaction can be varied over a very wide range by magnetically tuning the two-body scattering amplitude. For positive values of the s-wave scattering length" a" atoms with different spins are observed to pair into bound molecules which, at low temperatures form a Bose

Condensate [10, 11]. The molecular BEC state is adiabatically converted into a ultra cold Fermi gas with a < 0 and $K_F |a| << 1$, [12, 113], where standard BCS theory is expected to apply. In the cross-over region the value of $|a|$ can be orders of magnitude larger than the inverse Fermi wave vector K_F and one enters a new strongly correlated regime known as unitary limit. In dilute systems, for which the effective range of the interaction R is much smaller than the mean inter particle distance, $K_F R << 1$, the energy of the non-interacting Fermi gas is ε_{FG},

$$\varepsilon_{FG} = \frac{3}{10}\frac{\hbar^2 K_F^2}{m} \quad \ldots\ldots \quad (15)$$

For the ultra cold degenerate Fermi gases, recent work [14] gives that the energy per particle of a dilute Fermi gas is $\frac{E}{N} = \varepsilon_{FG}$ and the energy of a weakly attractive Fermi gas is given by,

$$\frac{E}{N\varepsilon_{FG}} = 1 + \frac{10}{9\pi} K_F a + \frac{4(11-2\log 2)}{21\pi^2}(K_F a)^2 + \ldots\ldots \quad (16)$$

In order to investigate what kind of phase transition such an assembly can undergo, we multiply the right hand side of equation (16) by the thermal activation factor $e^{-\frac{\varepsilon_{FG}}{KT}}$ and write the total energy as,

$$E = N\varepsilon_{FG}\left[1 + \frac{10}{9\pi} K_F a + \frac{4(11-2\log 2)}{21\pi^2}(K_F a)^2\right] e^{-\frac{\varepsilon_{FG}}{kT}} \quad \ldots\ldots \quad (17)$$

Now the specific heat can be obtained from equation (17) as,

$$C = \frac{\partial E}{\partial T} = \frac{\partial}{\partial T}\left\{N\varepsilon_{FG}\left[1 + \frac{10}{9\pi} K_F a + \frac{4(11-2\log 2)}{21\pi^2}(K_F a)^2\right] e^{-\frac{\varepsilon_{FG}}{kT}}\right\} \quad \ldots\ldots \quad (18)$$

$$C = N\varepsilon_{FG} A\left(-\frac{\varepsilon_{FG}}{k}\right)\left(-\frac{1}{T^2}\right)e^{-\frac{\varepsilon_{FG}}{kT}} = N\varepsilon_{FG}^2\,\frac{A}{kT^2}\,e^{-\frac{\varepsilon_{FG}}{kT}} \quad \text{..............................} (19)$$

Since $|K_F a| << 1$, the quantity A can be approximated as,

$$A \approx \left[1 + \frac{10}{9\pi}K_F a + \frac{4(11-2\log 2)}{21\pi}\left(K_F a\right)^2\right] \quad \text{...} (20)$$

Using the relation, $e^{-\frac{\varepsilon_{FG}}{kT}} = 1 - e^{-\frac{\varepsilon_{FG}}{kT}} + ... \approx 1 - e^{-\frac{\varepsilon_{FG}}{kT}}$ and neglecting higher terms in equation (19) gives,

$$C = \eta\,\frac{1}{T^2}\,e^{-\frac{\varepsilon_{FG}}{kT}} \quad \text{..} (21)$$

The quantity $\eta = N\varepsilon_{FG}^2 A/k$ is a constant. The following parameters were used to calculate the specific heat capacity, C and to plot the variation of C against T for temperature range $T = 0K$ to $T = 120K$

$K_F = 0.25$, $a = 10^{-6}$ and 10^{-8}, mass of electron, $m = 9.1\times10^{-24}$ gm, ε_{FG} is calculated from equation (15). The quantity $k = 1.38\times10^{-23}\,J/K$ is the Boltzmann constant

Results and Discussions

Figure 4.1 shows the specific heat dependence with temperature ranging from $0K$ to $120K$. The specific heat value approaches infinity at temperature $T = 120K$ pointing to a possible specific heat jump at this temperature

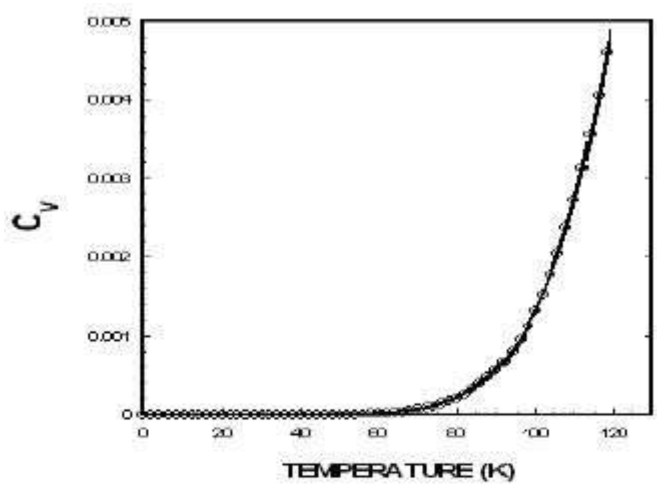

Figure 4.1: A graph of variation of the specific heat capacity, C_V *with the temperature for low temperature superconductors*

Figure 4.2 below shows the temperature dependence of specific heat of high temperature superconductors ranging from $90K$ to $180K$

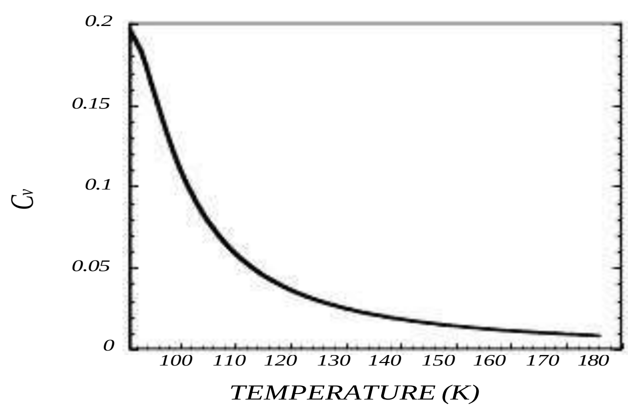

Figure 4.2: Graph of variation of specific heat capacity, C_V *with the temperature, T for high temperature superconductors.*

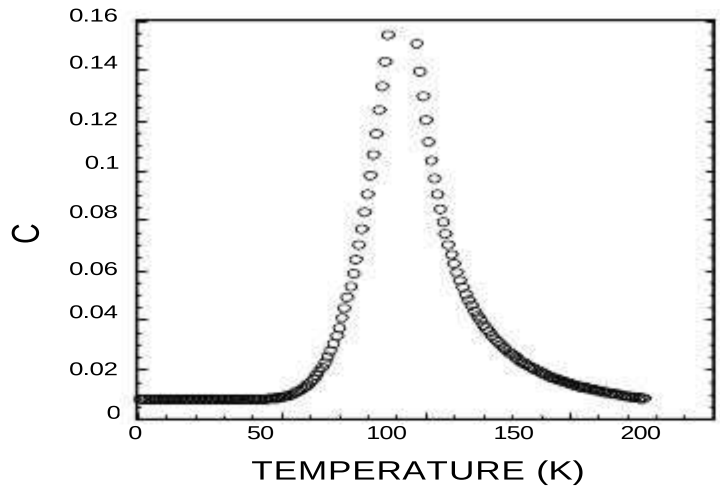

Figure 4.3: Graph of variation of specific heat capacity, C_V *with the temperature, T showing the heat jump.*

The specific heat jump due to the superconducting transition at about $90K$ is observed.

In this work we have investigated the specific heat capacity dependence with temperature for high temperature superconductors showing specific heat jump at the transition temperature $T_C = 90K$. Similar results were obtained in work done by Liu [15] on a possible second-order phase transition at which a gap opens in superconductors showing that there is a second-order phase transition at the temperature T_C.

The superconducting phase transition in heavy fermions $CeCoIn_5$ (T_C=2.3 K in zero field) becomes first order when the magnetic field $H_C(001)$ is greater than 4.7 T, and the transition temperature is below $T_0 \approx 0.31T_C$ [16]. The change from second order at lower fields is reflected in strong sharpening of both specific heat and thermal expansion anomalies associated with the phase transition.

Experimental data obtained from thermodynamic measurements in under doped high temperature superconductors [17] show unusual anomalies in the temperature dependence of the electronic specific heat both in the normal state and at the critical point associated to the superconducting phase transition. Based on a phenomenological description of the pseudo gap phase, analytical and numerical calculations were performed for the temperature dependence of the specific heat for both the superconducting and normal state. The reduced specific heat jump at the transition point was explained by a modified electronic single particle contribution to the specific heat in the presence of the normal state pseudo gap.

The specific heat $C_v(T)$ of iron-based high temperature superconductor $SmO_{1-x}F_xFeAs$ ($0 \leq x \leq 0.2$) was systematically studied [18]. For the undoped x=0 sample, a specific heat jump was observed at $T_C = 130K$. A simple consideration demonstrates that if the temperature of a second-order phase transition is suppressed by fluctuations, the dominating effect at the transition is a maximum, but not a jump of specific heat, C_v [19]

Conclusion

In conventional superconductors or BCS type superconductors, the superconducting transition is a second-order phase transition in the absence of the external magnetic field whereas the transition is of the first-order in a finite magnetic field. Whereas in high T_C superconductors [20], the situation is still not clear. In some materials, the superconducting transition seems to be of the first-order. In those materials in which the nearest neighbours, Coulomb repulsion V between the electrons in the copper oxide planes is sufficiently large, the transition is of first-order, whereas if V is less than some critical value V_C, the transition is of second-order. In recent study [6], the role of attractive interlayer and intralayer interactions in layered high T_C Cuprate superconductors have been investigated using a one- band two layer tight binding Hamiltonian. In another calculation [21] it has been shown that there is a finite specific heat jump at the transition temperature T_C, and hence the phase transition is of second-order

Phase transitions are of first order when the latent heat L = 0, and are of the second-order phase transition when there is a specific heat jump at the transition temperature T_C. In this study the variation of specific heat capacity with temperature for high temperature superconductors changes discontinuously but does not become infinite at T_C showing a finite specific heat jump at the transition temperature and hence the phase transition is of second order.

References

1. Onnes, H. K. "The resistance of pure mercury at helium temperatures". *Commun. Phys. Lab. Univ. Leiden* 12 (1911) 120.
2. Meissner, W. and R. Ochsenfeld. "Ein neuer Effekt bei Eintritt der Supraleitfähigkeit". *Naturwissenschaften* **21** (1933): 787.
3. Tinkham, M., Introduction to Superconductivity (2 *nd* ed.) (2004) Dover Books on Physics. 486-43503-2
4. *Larkin. A and A. Varlamov., Theory of fluctuations in superconductors (2005)* Oxford University Press, UK.
5. Anderson, P.W., Basic Notations of Condensed Matter Physics. (1997) Perseus Publishing.
6. Kashyap, A., S. C. Tiwari, A. Surana, R. K. Paliwal, S. L. Kakani. Theoretical Study of Specific Heat, Density of States, Free Energy, and Critical Field of High Temperature Cuprate Superconductors Based on Intra and Interlayer Interactions. Journal of Superconductivity and Novel Magnetism. 21 (2008) 29-143
7. Goldenfeld, N. Lectures on Phase Transition and the Renormalization Group. (1992) Perseus publishers.
8. Landau, L.D. and E.M., Lifshitz. Statistical Physics Part 1, Vol 5. Course of Theoretical Physics, 3rd ed (1994) Pergamon publishers.
9. Tilley D.R. and J, Tilley. Superfluidity and superconductivity. (2nd .ed.) (1986) Adam Hilger Ltd, Bristol.
10. Schroeder, M. R and W. H. Freeman Fractals, chaos, power laws: minutes from an infinite paradise (1991), Manfred Publication, New York.
11. Astrakharchik, G. E., Boronat, J., Casulleras, J. & Giorgini, S. “Superfluidity versus Bose Einstein condensation in a Bose gas with disorder,” *Phys. Rev. A* **66**, (2002) 023603-1.
12. Jochim S., Bartenstein M, Altmeyer A, Hendl G, Riedl S, Chin C, Hecker Denschlag J, Grimm R. Bose-Einstein condensation of molecules , Journ. Science. 302 (2003) 2101-3.
13. Greiner. M, C. A. Regal, and D. S. Jin. Emergence of a molecular Bose-Einstein condensate from a Fermi gas. Journ. Nature 426 (2003) 537.
14. Bartenstein M, A. Altmeyer, S. Riedl, S. Jochim , C. Chin, J. H Denschlag, R. Grimm. Collective excitations of a degenerate gas at the BEC-BCS crossover. Phys Rev Lett. 92: 20

(2004) 203201

15. Liu, F. S., W.F. Chen and K. Peng. "A possible second-order phase transition at the temperature at which a gap opens in superconductors". *J. Phys. Condens. Matter* **13** 2817 (2001)
16. Bianchi. A, R. Movshovich, N. Oeschler, P. Gegenwart, F. Steglich, J. D. Thompson, P. G. Pagliuso, and J. L. Sarrao. First-Order Superconducting Phase Transition in $CeCoIn_5$. Phys. Rev. Lett. 89, 137002 (2002)
17. Tifrea, I. and C. P. Moca. Specific heat behavior of high temperature superconductors in the pseudo gap regime. The European Physical Journal B. Condensed Matter and Complex Systems, 35(2003) 33-39
18. Ding, L., C. He, J. K. Dong, T. Wu, R. H. Liu, X. H. Chen, and S. Y. Li. Specific heat of the iron-based high- T_c superconductor $SmO_{1-x}F_xFeAs$. Phys. Rev. B 77, 180510 (2008).
19. Brazovskii, S., P. Monceau and N. Kirova. Distributed latent heat of the phase transitions in low-dimensional conductors. International Workshop on Electronic Crystals. J. Phys. IV France **131** (2005) 315-318.
20. Bang, Y., C. Castellani, K. Grilli, G. Kotliar, R. Raimondi, Z. Wang., Single Particle and Optical Gaps in Charge-Transfer Insulators. International Journal of Modern Physics B, 6 (1992) 531-545.
21. Khanna, K. M., S.M. Kirui, T. W. Sakwa, P. K. Torongey, Y. K. Ayodo, S. Rotich., Specific heat jump in anisotropic $YBa_2Cu_3O_{7-\delta}$ superconductor. Indian. J. Pure and applied physics 45 (2007)