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العدد العشرون
يناير 2022م

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Electronic Specific Heat of Multi Levels Superconductors Based on the BCS Theory

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Abstract:

In this work, the electronic specific heat as a function of temperature has been investigated using Bardeen, Cooper and Schrieffer theory (BCS). The electronic specific heat is obtained as a function of temperature by simplified derived equations based on the BCS theory and some concepts of statistic mechanics. Analyzing the obtained equations has shown that the electronic specific heat has an exponential term and it vanishes rapidly (as $\exp(\frac{\Delta}{k_B T})/T^2$) at low temperature. In addition, it confirms that there is a gap in the distribution of energy levels available to the electrons in a superconductor. Numerical calculations based on the derived equations have been applied for systems of two, three and four levels using maple software and the obtained results are reported in this paper.

Keywords: *Superconductors, specific heat, BCS theory, energy gap, statistical mechanics.*

Introduction:

Superconductivity is a peculiar phenomenon in condensed matter physics where electrons condense in so-called Cooper pairs can move freely in the materials giving rise to interesting physical properties. There are two main characteristics of superconducting state; First, the resistance is always zero below a certain critical temperature $T_c^{[1]}$ as

shown in figure (1.a). Second, in the superconducting state, the magnetic flux is expelled completely to the exterior as shown in figure (1.b).

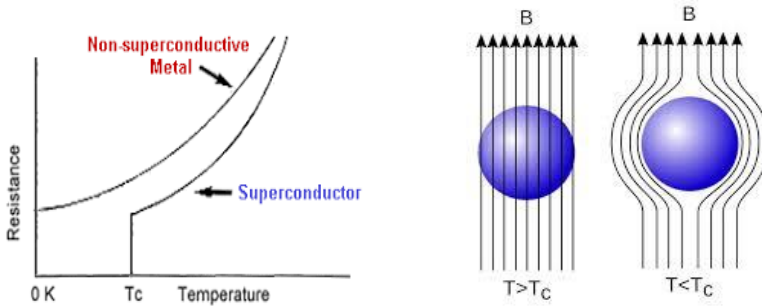


Figure (1) Resistivity as a function of temperature and Meissner effect for superconductors ^[1,2].

This phenomenon was observed by Meissner and Ochsenfeld and it is usually known as Meissner effect ^[2], as shown in figure (1.b). The thermodynamic properties of superconductors are determined mainly by the electron-phonon interaction. The electron-phonon interaction is able to couple two electrons in a way that they behave as if there is a direct interaction between them. In this case, one electron emits a phonon, which is then immediately absorbed by the other. This emission and subsequent absorption of a phonon could give rise to weak attraction between the electrons of the type, which might produce an energy gap ^[3]. The energy gap of a superconductor is different from a semiconductor energy gap. From the band theory, energy bands are a consequence of the static lattice structure. In a semiconductor, energy bands describe the range of energy levels that electrons may occupy, as well as the range of energy that they cannot occupy which is known as energy band gaps. Therefore, the energy gap in a semiconductor is the energy required to excite electrons from the top of the valence band to the bottom of the conduction band. On the other hand, in the superconductor, the energy gap is the energy required to excite electrons from the ground state (Cooper pairs) to the excited state. This means the energy gap of a superconductor is the energy required to break up a pair of electrons. Whereby Cooper pair electrons are bounded by an energy 2Δ , as shown in figure (2) ^[3,4].

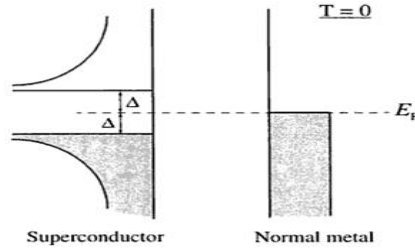


Figure (2) The density of states near the Fermi level E_F in a superconductor, showing the energy gap 2Δ at $T = 0$, and in a normal metal^[4].

Specific heat is a powerful tool to investigate the physical properties of superconductor materials. Changes in specific heat as a function of temperature associate various types of phase transition, (structural, electronic, magnetic...) with a function of a physical quantity like temperature or magnetic field. In addition, specific heat is related to several thermodynamic quantities like entropy, internal energy and free energy, which are important properties to investigate superconducting materials behavior^[5].

Successful microscopic theory of superconductivity was originally, given by Bardeen- Cooper-Schrieffer (BCS) in 1957. This theory is based on the condensation of electrons into pairs known as the Cooper pairs through electron-phonon interaction. There are two interactions in the superconducting state, the electron-phonon interaction that describes the formation of these pairs and the coulomb interaction between pairs of electrons. There are many parameters provided by this theory such as the critical temperature T_c , energy gap Δ , electron-phonon coupling λ , critical field H_c , and specific heat that shows how to treat the superconducting phenomena^[6].

At very low temperature ($T \rightarrow 0K$), the BCS theory predicts that the energy gap 2Δ can be written as^[7]:

$$2\Delta(T \approx 0) = 3.52 K_B T_c \quad (1)$$



And ,

$$\Delta(T \approx T_c) \approx 3.06K_B T_c \left(1 - \frac{T}{T_c}\right)^{1/2} \quad (2)$$

where K_B is Boltzmann's constant (1.38×10^{-23} joule per Kelvin),

$$\frac{\Delta(T)}{\Delta(0)} \approx 1.74 \left(1 - \frac{T}{T_c}\right)^{1/2} \quad , \quad T \approx T_c \quad (3)$$

The ration between $\Delta(T)$ and $\Delta(0)$ as a function of T/T_c , has been investigated theoretically and experiementally. The obtained experiemental results have agreed with the theoretical prediction by the BCS theory, whereas both of them have shown similar behaviour at weak coupling limit. This relation is indicated in figure (3).

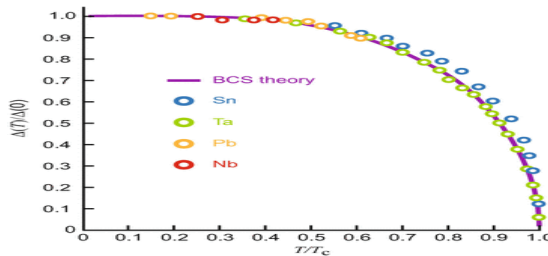


Figure (3) Temperature dependence of energy gap in the BCS theory and experiement ^[8]. Although this universal curve holds only in a weak coupling limit, it is a good approximation in most cases ^[7].

The critical temperature T_c depends on several parameters including the density of state at Fermi surface $N(\epsilon_F)$, the effective net pairing potential for electron- phonon interaction V_0 and typical energy transferred

in scattering with the lattice, $\hbar\omega_D = K_B\theta_D$ where θ_D , ω_D are the Debye temperature and Debye frequency respectively ^[3,9].

$$K_B T_c = 1.13 \hbar \omega_D e^{-1/N(\epsilon_F)V_0} \quad (4)$$

The BCS theory identifies the superconducting transition temperature T_c in terms of Debye temperature θ_D by the equation:

$$T_c = 1.13 \theta_D e^{-1/N_0 V_0} = 1.13 \theta_D e^{-1/\lambda} \quad (5)$$

Where $\lambda = N_0 V_0$, N_0 is the density of states at Fermi level ^[9].

When a system is supplied with a small amount of heat, some of the energy is used to increase the lattice vibrations and the remainder is used to increase the energy of the conduction electrons. Therefore, the specific heat of a solid system is mainly dominated by contributions from phonons and electrons.

The total specific heat of a system is a sum of two components, electronic specific heat C_e and lattice specific heat C_{ph} . Specific heat measurements give information on the electron-phonon coupling λ , which help to ascertain the role of phonons in the superconductivity and help to characterize the phonon contribution to the temperature-dependent resistivity. The electronic specific heat C_e of the electrons represents the ratio of that portion of the heat used by the electrons to the rise in temperature of the system ^[10, 11].

Variations of C_e in a superconductor material as a function of the absolute temperature T in the normal and in the superconducting state are shown in figure (4). The figure indicates an abrupt change in C_e at T_c occurs in superconducting state, while a linear change appears in the normal state. In addition, the electronic specific heat in the superconducting state C_{es} is smaller than in the normal state C_{en} at low



enough temperatures. However, C_{es} becomes larger than C_{en} as the transition temperature T_c is approached, where by it drops abruptly at T_c [3].

In the zero magnetic field, the BCS theory also predicts the electronic component of the specific heat C_{es} , at low temperature contains exponential term [3,12], since

$$C_{es} = \gamma T_c 1.34 \left(\frac{\Delta_0}{T}\right)^3 / 2 e^{\frac{\Delta_0}{k_B T}} \quad (6)$$

Where γ is the coefficient of the linear term in the normal state. The BCS theory also predicts a discontinuity at T_c of tude: $\frac{C_{es} - C_{en}}{C_{en}} \Big|_{T_c} = 1.43$.

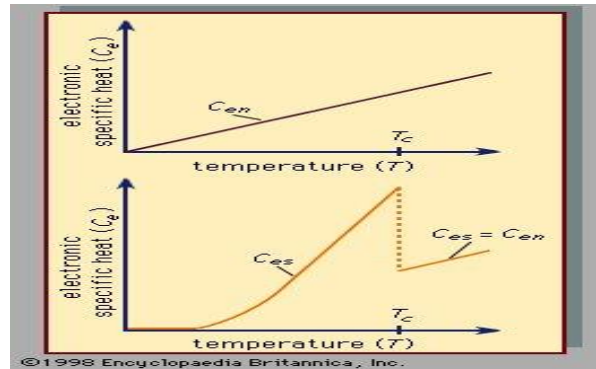


Figure (4) Electronic specific heat variations of a superconductor in normal and in superconducting state as temperature is approaching T_c [3].

Superconducting-state properties of MgB_2 were characterized by thermodynamic measurements [11]. The obtained results indicate existing multiple values of energy gaps. The electronic specific heat C_e was obtained experimentally for the iron-based superconductor $BaFe_2(As_{0.68}P_{0.32})_2$. It was found an exponential-like behavior [14], and this result was confirmed by others [11,15].

In this work, the BCS theory has been applied to evaluate energies e and four levels as a function of energy gap Δ , and the partition func-



tion has been used to derivate specific heat function as will be indicated below;

Theory and Method:

The BCS theory indicates that Cooper pair electrons are bounded together by an energy 2Δ . Each time a pair is broken, an amount of energy is at least as much as the energy gap (Δ) must be supplied to each of the two released electrons in the pair so, an energy at least as twice as great (2Δ) must be supplied to the superconductor.

According to the BCS theory, for two levels system, the energies will take values from zero to Δ , while for three levels system will be $0, \Delta, 2\Delta$ and four levels system, the energies values $0, \Delta, 2\Delta, 3\Delta$ and so on.

The partition function for a system is simply an exponential function of the sum of all possible energies for that system. It is assumed that the different energies of any particular state can be separated.

In statistical mechanics, a partition function Z for a system of fermions with a superconductive attractive interaction can give by form;

$$Z = \sum_{r=0}^{\infty} e^{-\beta \varepsilon_r} \quad (7)$$

For two levels system, $\varepsilon_0 = 0$ and $\varepsilon_1 = \Delta$ so equation (7) can be written as

$$Z = 1 + e^{-\beta \Delta} \quad (8)$$

The average energy \bar{E} of this system which identified by:

$$\bar{E} = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} \quad (9)$$

$$\bar{E} = \frac{\Delta}{1 + e^{\beta \Delta}} \quad (10)$$



The specific heat at constant volume can be given by the relation;

$$C_v = \left(\frac{\partial E}{\partial T}\right)_v = \frac{\partial E}{\partial \beta} * \frac{\partial \beta}{\partial T} \quad (11)$$

Where $\beta = \frac{1}{K_B T}$, then equation (11) can be written as:

$$C_v = -\frac{1}{K_B T^2} \frac{\partial E}{\partial \beta} \quad (12)$$

$$= -\frac{1}{K_B T^2} \frac{\partial}{\partial \beta} \left(\frac{\Delta}{1 + e^{\beta \Delta}} \right) \quad (13)$$

Therefore, the specific heat per one particle at constant volume is;

$$C_v = \frac{\Delta^2}{K_B T^2} \frac{e^{\beta \Delta}}{(1 + e^{\beta \Delta})^2} \quad (14)$$

For N particles and subsisting $\beta = \frac{1}{K_B T}$, specific heat as a function of temperature T can be formed as

$$C_v = \frac{N \Delta^2}{K_B T^2} \frac{e^{\frac{\Delta}{K_B T}}}{(1 + e^{\frac{\Delta}{K_B T}})^2} \quad (15)$$

For 3 levels system $\epsilon_r = 0, \Delta, 2\Delta$

$$Z = 1 + e^{-\beta \Delta} + e^{-2\beta \Delta} \quad (16)$$

Substituting the above equation into Eq. (9) we can get



$$\bar{E} = \frac{\Delta(2+e^{\beta\Delta})}{1+e^{2\beta\Delta}+e^{3\beta\Delta}} \quad (17)$$

Using Eq. (12), specific heat can be formed as

$$\frac{C_v}{K_B} = \left(\frac{\Delta}{K_B T}\right)^2 \frac{(e^{\beta\Delta}+4e^{2\beta\Delta}+e^{3\beta\Delta})}{(1+e^{\beta\Delta}+e^{2\beta\Delta})^2} \quad (18)$$

$$\frac{C_v}{K_B} = N \left(\frac{\Delta}{K_B T}\right)^2 \frac{(e^{\frac{\Delta}{K_B T}}+4e^{2\frac{\Delta}{K_B T}}+e^{3\frac{\Delta}{K_B T}})}{\left(1+e^{\frac{\Delta}{K_B T}}+e^{2\frac{\Delta}{K_B T}}\right)^2} \quad (19)$$

For 4-levels system $\epsilon_r = 0, \Delta, 2\Delta, 3\Delta$

$$Z = 1 + e^{-\beta\Delta} + e^{-2\beta\Delta} + e^{-3\beta\Delta} \quad (20)$$

So, specific heat for N particles

$$\frac{C_v}{K_B} = N \left(\frac{\Delta}{K_B T}\right)^2 \frac{(e^{\frac{\Delta}{K_B T}}+4e^{2\frac{\Delta}{K_B T}}+10e^{3\frac{\Delta}{K_B T}}+4e^{4\frac{\Delta}{K_B T}}+e^{5\frac{\Delta}{K_B T}})}{\left(1+e^{\frac{\Delta}{K_B T}}+e^{2\frac{\Delta}{K_B T}}+e^{3\frac{\Delta}{K_B T}}\right)^2} \quad (21)$$

Results and Discussion:

The obtained electronic Specific heat curves for the studied energy levels are plotted in figures (5, 6, 7). The curve of the two-levels system, shows a cusp shape near the transition temperature. This curve can be investigated as following: At low temperature ($T \rightarrow 0$), Cooper pairs will be at the ground state and the energy gap is given by $\Delta(T) \approx 3.06K_B T_c(1 - \frac{T}{T_c})^{1/2}$, so $e^{\frac{\Delta}{K_B T}} \gg 1$, and $C_v(T) \sim (\exp(-\frac{\Delta}{K_B T}))/T^2$. While at high temperature ($T \rightarrow \infty$), Cooper pairs are broken and re-



leased electrons will move from ground state to excited states, also $\Delta \approx 0$ at $T \approx T_c$, this leads to that $e^{\frac{\Delta}{k_B T}} \approx 1$, and $C_v \sim 1/T^2$. This means, the electronic specific heat will vanish with increasing temperature.

In addition, electronic specific heat for systems with two, three and four-levels plotted in figures (5-7) show its decay exponentially with decreasing temperature. All the results show that due to the energy gap, the electronic specific heat of the superconductor is suppressed strongly at low temperature, whereby no thermal excitation left. For a system with an energy gap, no more energy is needed to heat it up than heating up a normally conductive system with continuous energy.

For a gapped quantum system at a temperature far below the energy gap Δ , it is expected that the thermal mixture to be almost entirely in the ground state, with exponentially small weighting for excited states. So the expected energy E is effectively quantized and pinned down to its ground state. The system can only absorb a quantized amount of energy Δ , so if the system in the ground state and has been put into thermal contact with a bath at any temperature $T \gg \Delta$, the system basically doesn't absorb any amount of energy at all until $T \sim \Delta$, so $\frac{\partial E}{\partial T} = 0$, below that temperature. As a result, specific heat is exponentially suppressed. More precisely, if $T \gg \Delta$, we expect that all excited states above the first one will contribute negligibly.

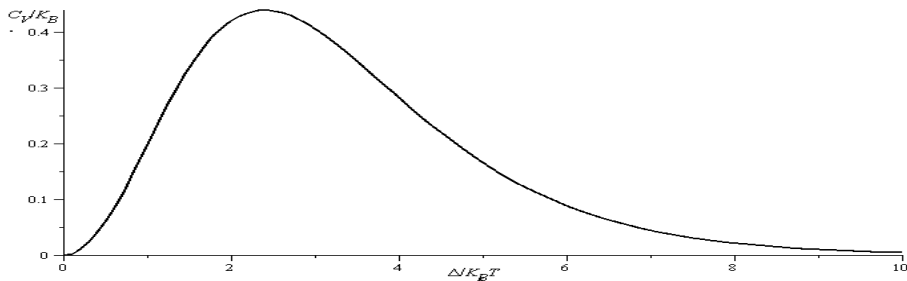


Figure (5) Electronic specific heat of 2-levels system as a function of temperature.

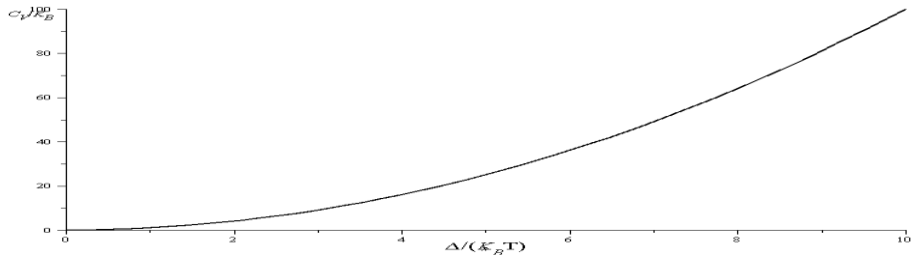


Figure (6) Electronic specific heat of 3-levels system as a function of temperature.

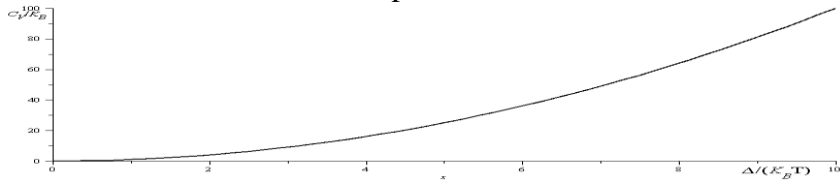


Figure (7) Electronic specific heat of 4-levels system as a function of temperature.

Conclusion:

The electronic specific heat is obtained by differentiating the average energy E of system with respect to the absolute temperature T using the relation $C_v = \left(\frac{\partial \bar{E}}{\partial T}\right)_v$. For systems with n levels, the BCS theory describes the energies of these levels as a function of energy gap Δ with values $\epsilon_r = 0, \Delta, 2\Delta, 3\Delta, \dots$. Obtained results have shown that; at low temperature, the electronic component of the specific heat depends on the absolute temperature. While at room temperature, it is completely negligible. Electronic specific heat dependence on temperature indicates presence of low energy excitations.

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