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A Simple Mechanism for Superconductivity

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Author's contribution

The sole author designed, analyzed and interpreted and prepared the manuscript.

Article Information

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Short Research Article

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ABSTRACT

Based on the statistical thermodynamics and quantum mechanics, a simple mechanism for superconductivity has been proposed. With the method described in this paper, the transition temperatures can be easily determined, as a result, the efficiency in searching new superconductivity material is greatly improved.

Keywords: Superconductivity; transition temperature; cooper pair.

1. INTRODUCTION

The topics regarding the mechanism of the material conductivity becomes hot due to the discovery of the high temperature superconductivity [1]. Till now, several Nobel Prizes are awarded to the researchers in this field [2]. The most famous theory about the superconductivity is the BCS theory [3], of which the founders are awarded Nobel Prize for their theoretical contribution to science. However, with new superconductivity materials being discovered, the more and more experimental results can't be explained by the BCS theory, therefore, the different mechanisms about the superconductivity are proposed and the new theories are developed. The most recent ones are the resonating-valence-band theory [4] and the spin fluctuation theory [5]. Our question is which one is correct? Maybe most of these superconductivity theories just catch a part of the facts about the superconductivity? For example, the BCS theory demonstrates the cooper pairs are formed in the superconductivity materials but no direct evidence shows that the cooper pairs take response for the superconductivity, not mention to assign the formation of the cooper pairs as unique mechanism for the superconductivity of materials. The question is whether there exists a general mechanism for the superconductivity? In this paper, based on the statistical dynamics and quantum theory, we would like to make our effort toward a general mechanism for the superconductivity.

2. THEORY

Fig. 1 illustrates the basic situation in the materials. The electron density in the potential well is n(e). If the electron moves out of the potential well, then the electron makes contribution to the conductivity of materials, otherwise, the contribution of electron to the conductivity of materials is zero. In order for electron to move out of the potential well, the electron must overcome the energy barrier. If the electron is bounced back or scattered back by the energy barrier, the electron makes no contribution to the conductivity of materials. It is obvious that if this energy barrier in some way is reduced, the conductivity of materials will increase: if this energy barrier totally disappeared, then the electron can move freely in the materials and the materials become superconductivity, therefore, the energy barrier is the key factor which determines the material behavior as insulator, semiconductor, conductor or superconductor.

From the statistical thermal dynamics and quantum mechanics [6], there are four main factors responsible for the formation of the energy barrier. One is the lattice vibration, called phonon. The stronger the lattice vibration (E_{vib}) , the higher the energy barrier $(E_{vib}-E_e)$ and therefore, the more chance for the electron being scattered back by the energy barrier $(E_{vib}-E_e)$; Second is the coulomb attraction from the nuclei, the stronger the attraction, the higher the energy barrier (E_{vib}-E_e) becomes and the more difficult for the electron to move in the materials; Third is the energy level of electron in the materials. The higher the energy level of electron, the lower the energy barrier (Evib-Ee) becomes and easier for the electron to move in the materials; Fourth is the magnetic interaction which makes the movement of electron in the materials more difficult, therefore, increases the energy barrier (E_{vib}-E_e).In fact, the last three factors are included in the binding energy term (E_e).

Based on these understandings, the probability for the electron to pass the energy barrier (E_{vib} - E_e) or tunnelling through the energy barrier (E_{vib} - E_e) can be written as:

$$P = A \exp \frac{-(E_{vib} - E_e)}{RT} n_e \tag{1}$$

Where
$$E_{vib} = 9N(\frac{k_BT}{hv_D})^3 k_b T \int_0^{x_m} \frac{x^3}{e^x - 1} dx$$

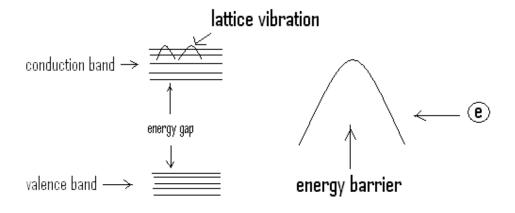


Fig. 1. Illustration of electron moving in the meta

$$x = \frac{hv}{k_BT}$$
 and $x_m = \frac{hv_D}{k_BT}$
 $E_e = \gamma T^2$, $\gamma = \frac{Rk_B\pi^2}{4E_e}$, n_e =density of

electron,

Then,

$$C_{vib} = \frac{\partial E_{vib}}{\partial T} = 9R(\frac{T}{\theta_D})^3 \int_0^{x_m} \frac{x^4 e^x}{(e^x - 1)^2} dx$$
(2)

Where $\theta_D = \frac{hv_D}{k_B}$

and

$$C_e = \frac{\partial E_e}{\partial T} = \frac{Rk_B \pi^2}{2E_f} T = 2\gamma T$$
(3)

Then

$$C_{total} = C_{vib} + C_e = 9R(\frac{T}{\theta_D})^3 \int_0^{x_m} \frac{x^4 e^x}{(e^x - 1)^2} dx + 2\gamma T$$
(4)

P is the probability of electron passed the energy barrier; A is the pre-exponential factor; R is the mole constant; T is the absolute temperature; k_B is the Boltzman constant; h is the Planck constant; v is the lattice vibration frequency; v_Dis the cutoff frequency of the lattice vibration, E_f is the Fermi energy, E_{vib} is the total lattice vibration energy; E_e is the total electron energy; C_{vib} is the total heat capacity from the lattice vibration; C_e is the total heat capacity of electron; θ_D is Debye temperature. Due to the derivation of E_{vib}, E_e, C_{vib} and C_e can be found easily in the most of physical chemistry books [6], therefore, we don't repeat here.

There are four cases.

Case 1. E_{vib} >> E_e , then the materials will show as insulator. The electron tunnelling probability is too small to be accounted. Most of insulators belong to this category.

Case 2. E_{vib} > E_e , then the materials will show certain conductivity but not good conductor. The temperature has great influence on the conductivity of these materials. Increasing the temperature, the conductivity of materials increases.

Case 3. E_{vib} - E_e = ϵ , where ϵ is the smallness, then the materials will show good conductivity. Most of metal belong to this category. Since E_{vib} and E_e are temperature dependent, therefore, the conductivity of materials also depends on the temperature. How the conductivity of materials changes with temperature depends on the temperature coefficient of E_{vib} and E_e . For metal, increasing the temperature, contrarily to the situation in case 2, the conductivity of materials decreases.

Case 4. E_{vib} << E_e , then the materials will show the superconductivity. That means the electron in the materials can move freely like free electron. Here we don't need the concept of the cooper pair formation.

To our knowledge, no materials show the superconductivity at room temperature. From the discussion above, Evib and Ee are all temperature dependent, which offers the possibility for the to meet the requirement materials of superconductivity by changing the temperature. In fact, till now, the discovered superconductors are always realized experimentally by reducing the temperature of materials to extremely low temperature, then the condition in case 4 above is met. That is to say, with decreasing the temperature, the E_{vib} decreases faster than E_e. Therefore, the energy barrier $(E_{vib}-E_e)$ is effectively reduced. This result opens a new way for us to synthesize the new superconductivity materials and determine what kinds of materials potential are the candidate for the superconductivity materials. Furthermore, from C_{vib} T and C_{e} T, we also can determine the critical temperature of materials for superconductivity (Fig. 2, see appendix).

Normally, E_{vib} always increases with temperature, but this temperature dependence of E_{vib} is not linear, therefore, it is possible in certain range of temperature, the Ee will increase faster than E_{vib}, then principally, we can also observe the superconductivity of materials by increasing the temperature of materials. An extremely case is to increase the temperature of materials so high that the materials become plasma. Nobody doubt the superconductivity of plasma but also nobody believe the superconductivity of plasma coming from the formation of the cooper pair in plasma. Obviously, the superconductivity of materials doesn't need the cooper pair concept here.

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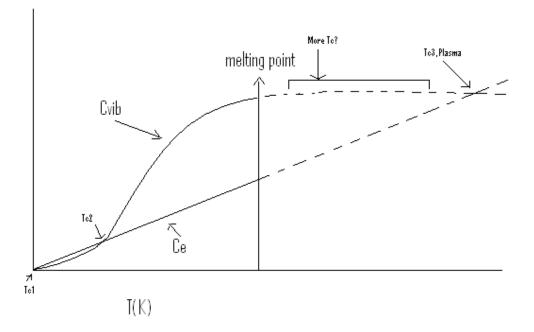


Fig. 2. Illustration for determining the transition temperature

From Fig. 1, we see that compared to E_{vib} , the position of valence band is too low to make the condition in case 4 to be met. Whereas the conduction band is at right position which can meet the condition in case 4 by changing the temperature of materials.

From the discussion above, $E_{vib}=E_e$ is the requirement for the transition of the normal material to superconductor. Based on the expressions of E_{vib} and E_e , principally, we can determine at least two transition temperature for most of materials. One is at extremely low temperature as most of researchers focused on at present; another is at very high temperature at which most of materials will become plasma (Fig. 2).

(Table 1) listed the T_c determined with method described above and Fig. 2 illustrates how to determine the T_c from $C_{vib-}T$ and $C_{e-}T$. In fact, we can get at least three T_cs . Two of them is at low temperature; one at high temperature. For $T_c=0K$, there is no practical meanings because the absolute zero temperature can't be realized. But theoretically we can say there exists another superconductivity phase at T=0K, which is different from the $T_c\approx 0.1_140K$ superconductivity phase. For the high temperature T_c , it is far

beyond the melting temperature of element listed in the (Table 1). This gives us a hint, that is, at high temperature, there may exist one or more superconductivity phases. To my knowledge, one superconductivity phase definitely exists, that is the plasma. Whether there exists other superconductivity phase or not, we still need doing experiment to verify but the equation we developed above should be modified before applying to the high temperature phase because the material is not solid under such high temperature. However, following our work here, it should be easier to setup new equations for $C_{vib-}T$ and $C_{e-}T$, then the concept developed here is still valid.

From the (Table 1), we noticed that the difference exists between the data in this work and that in the literature [7,8]. We think this deviation comes from the two sources. One is the too simple model for us to get the expression for heat capacity of electron (free electron gas model). In order to correct this drawback, some researchers suggest the concept of the effective mass for electron in the calculation [9]. In our following work, we will try some different model to improve our calculation; another is the experimental data comes from the different form of samples, such as film and powder. Even for

the experimental data, some literature only can give the range of transition temperature instead of the exact value [7,8]. In a word, as a first step, our data are still in the acceptable range of experimental data. In (Table 1), we also noticed that the transition temperatures are far from the temperature, therefore, room the wide applications of the superconductors are prohibited. The task of the researchers is to find the materials of which the transition temperatures are not too far from the room temperature. Our work here offers an easy way to find the material requirement of meeting the transition temperature for superconductivity, that is, by drawing C_{vib} T and C_{e} T to determine the possible transition temperature of materials for superconductivity. This kind of research can be done by the cooperation between synthetic scientist and the theoretical scientist. For example, the theoretical scientist can design the materials which have certain crystal structure and determine what kind of material is possible to have the adequate transition temperature for superconductor, the synthetic scientist can synthesize the material in Lab and measure the C_{vib} T and C_{e} T. In this way, we can greatly save the time and reduce the cost in searching new superconductivity materials.

It should be pointed out that the equations of E_e and Ce above are developed from the free electron gas model, the free electron gas model⁶ is oversimplified model to describe the behavior of electron in metal, therefore, if the electron behavior deviated from the free electron gas model, the big difference in transition temperature will occur between our calculation result and experimental data. For example, Be in the Table 1 has two electron paired in 2s orbital, which make Be more like non-metal instead of metal, therefore, the calculation result in this work based on free electron gas model deviate greatly from the data in literature. In order to overcome this defect, some researchers propose to use the effective electron mass in the calculation [9]. In fact, we also can follow the method 3 in appendix to determine the Ce experimentally, then, following the same procedure, we can determine the transition temperature of matter. This is especially a good way for those systems which lack of adequate model to describe the electron behavior, such as oxide. Our following work will focus on this kind of system and will present the result later.

Xu; BJAST, 5(6): 580-587, 2015; Article no.BJAST.2015.056

Table 1. Transition temperature (T_c/K)

FelementTc1(K)Tc2(K)Tc3(K)Tc1(K)Tc2(K)Tc3(K)Tc4(K) in reference [7-8]Li05.715552[7-8]Na01.618190[7-8]Na00.912058[7-8]Rb00.912058[7-8]Rb00.510390[7-8]Cu03.336122[7-8]Aq02.634335[7-8]Au07.1187851.175Be018.01198410.026Mg06.619483[7-8]Ca02.47036[7-8]Ba01.4.49320[7-8]Sr02.47036[7-8]Ba01.4.33394[7-8]Mn018.02989[7-8]Zn03.332150.85Cd01.8363030.517Hg(β)00.7182753.949Ga03.332150.46Mn01.0149983.408Ti00.13.17231.96Sin01.7182753.949Ga01.7182753.949Ga01.7317831.96Sin01.181177.196Sin01.181177.196Sin01.181271.92 </th <th></th> <th></th> <th></th> <th>•</th> <th></th>				•	
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Changing the temperature of materials is a conventional but not the best way to change the properties of materials, such as electric and heat conductivity. For example, when we reduce the temperature of materials, Evib decreases but at the same time, E_e also decreases, the net result is the energy barrier (E_{vib}-E_e) may not change. The decrease of E_{vib}, as discussed above, is good for the movement of the electron in the materials but the decrease of Ee is not good for the electron movement in the materials. If we increase the temperature of materials, Ee will increase, which is good for the electron movement in the materials but Evib will also increase in this case, which is not good for the electron movement in the materials. These two factors have counter influence on the conductivity of materials. This is one of the reasons why the superconductivity of materials only can be observed at extremely low or high temperature.

From the expressions of E_{vib} and E_e and Fig. 1, we also think the possibility to find a way just to promote the electron to high energy level but has no or minor influence on the E_{vib} , or reduce the E_{vib} effectively but has no or minor influence on E_e , then the energy barrier (E_{vib} - E_e) for the electron moving in the materials will be greatly reduced. In fact, we find the microwave is a potential method for this purpose, that is, the microwave can promote the electron to high energy level quicker but has less influence on E_{vib} for metal. The experimental result will be presented soon later. Another possible way is to change the pressure applied onto the materials, which we will explore in the future.

Here we would like to make some comment on the current superconductivity theory. The famous one is the BCS theory which supposes the superconductivity of material coming from the formation of the cooper pair of electron in the materials. In fact, no evidence shows that the paired electron can move faster or smother than a single electron or unpaired electron. In metal, all electrons in valence band are paired but they make almost no contribution to the conductivity of material, not mention to the superconductivity of materials (based on the quantum mechanics, the inner electrons still can make minor contribution to the conductivity of materials through tunnelling mechanism, but this contribution is too small to be accounted). Our work here also reveals that the superconductivity of materials mainly contributed by outer electron or conduction band electron because the requirement of $E_{vib} \le E_e$ is easier to meet, whereas for inner electron or valence band electron, the requirement of $E_{vib} \le E_e$ is difficult to meet.

3. SUMMARY

We setup a simple physical picture to show how the transition from the normal materials to superconductor happens and offer an easy way to determine the transition temperatures of materials for the superconductivity. Our work also point out there are three ways to reduce the energy barrier to meet the requirement of E_{vib}≤E_e. One is to reduce the temperature of material, which is to reduce E_{vib}, just as most of researchers are doing currently; second is to increase the temperature of materials. If Ee increase faster than E_{vib}, then the energy barrier (Evib-Ee) also can be effectively reduced, therefore, E_{vib}≤E_e can be met; third is to find a way to promote the electron in materials to high energy level but has no or minor influence on E_{vib} , then $E_{vib} \le E_e$ also can be realized. For some materials, the microwave can be applied for this purpose. Finally, our work also gives a clue for both synthetic scientist and theoretical scientist. For synthetic scientist, they can synthesize the materials which has certain crystal structure to meet the requirement of E_{vib}≤E_e, whereas for theoretical scientist, they can design or predict the materials which has certain crystal structure to meet the requirement of E_{vib}≤E_e. Our work makes the research much easier than before for scientist in searching the new superconductivity materials and avoiding randomly trying and error, therefore, improving efficiency and reducing the cost in searching the new superconductivity materials.

4. CONCLUSION

In this work, a simple, general mechanism for superconductivity has been setup which can greatly improve the efficiency in searching the new superconductivity materials in the future.

COMPETING INTERESTS

Author has declared that no competing interests exist.

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APPENDIX

Appendix

Here we offer three basic methods to calculate the transition temperature.

Method 1: Approximate Calculation

From the expression of C_{vib} (eq.(2), we know that the integration in the equation (2) is nonintegrated, as a result, no analytical solution for C_{vib} can be got, therefore, we only can get the result under certain approximation. Following the literature⁶, at temperatures much less than the Debye temperature, the equation of C_{vib} (eq.2) becomes

 C_{vib} =1.944x10³(T/ ϑ_D)³ J.mol⁻¹K⁻¹ which hold at T< ϑ_D /10. For T> ϑ_D /10, C_{vib} =464.45(T/ ϑ_D)³. In Table 1, all data are calculated using these approximate expressions of C_{vib} here.

Method 2. Numerical Calculation

If we hope to get more exact result than that in method 1, we have to use the numerical

calculation method. That is, change the integration in C_{vib} expression (eq.2) to summation expression, then, $C_{vib}=9R(T/\vartheta_D)^3$ $f(x_i), where f(x_i)=\sum_{i=1}^{i=n}\frac{n^4x_i^4}{(e^{nx_i-1})(e^{nx_i-1})}e^{nx_i}\frac{x_m}{n}$. Based on the same principle in Method 1, the transition temperature can be calculated.

Method 3. Experimental Method

From the expression of $C_{\mbox{total}}$ (see eq.4), we have

$$C_{total}/T = (C_{vib} + C_e)/T$$

= $9R(\frac{T}{\theta_D})^2 \int_0^{x_m} \frac{x^4 e^x}{(e^x - 1)^2} dx$
 $/\theta_D + 2\gamma$

 C_{total} is easier to be measured experimentally, therefore, by drawing $C_{total}/T \sim T^2$, then the intercept is 2γ . Then $C_{vib} = C_{total} - 2\gamma T$, therefore, we can determine the transition temperature by drawing $C_{vib} \sim T$ and $C_e \sim T$.

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