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Group Theory Explanation of Microscopic Superconductivity Theory

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Abstract:

In 1911, Dutch physicist Onnes discovered that after liquefying helium gas. At around 15 K, the resistance of mercury drops sharply to zero, which is named superconductivity and marks the beginning of human research on superconductors. So far, over a hundred types of superconducting materials have been discovered. With the discovery of superconducting materials and phenomena, many theoretical models have emerged to explain superconducting phenomena, promoting human understanding of condensed matter micro magnetism and other fields. Group theory is a mathematical concept. In mathematics and abstract algebra, group theory studies the algebraic structure of groups. In the study of physics and chemistry, many different physical structures, such as crystal structures and hydrogen atomic structures, can be modeled using group theory methods. So group theory and related group representation theory have a lot of applications in physics and chemistry. This article will elaborate on the phonon model that explains superconductivity theory, Cooper's model. And attempt to construct a model using molecular point group crystal dynamics knowledge to explore micro superconducting phenomena and theories.

Keywords: Micro superconductivity, Group representation theory, Cooper pairs, Phonons

1. Introduction

The exploration of superconducting materials by humans has a history of one hundred years. In 1911, Dutch scientist Onnes discovered that the resistance of mercury suddenly dropped to 0 at 4.2K. Such materials have strong current carrying capacity and low losses, and can be widely used in the field of electrical engineering. For over a hundred years, humanity has never stopped exploring superconducting materials, mainly searching for materials with high critical temperatures and high critical currents. In the 1980s, metal oxides became one of the most promising superconducting materials. In 1987, American scientist Zhu Jingwu and Chinese scientist Zhao Zhongxian successively developed the superconducting material yttrium barium copper oxygen (YBCO), which can reach a critical temperature of 90K (later proven to reach 100K), and metal oxidation entered the public eye from then on.

Since Onnes discovered superconductivity in 1911, a wealth of knowledge has been accumulated from experiments to macroscopic phenomenological theory.[1]

2. Superconducting theory

2.1 The lattice structure remains unchanged before and after superconducting phase transition

Firstly, experimental results have shown that the lattice structure remains unchanged before and after the superconducting phase transition, which proves that the superconducting phase transition is not caused by the lattice. Therefore, the superconducting phase transition only involves changes in the state of the electron gas.

2.2 Electron phonon interaction

Superconducting states have energy gaps, with a size of 2 Δ. The size of a material's energy gap can reflect its superconductivity. In the PIppard coherence length experiment, it can be observed that the arrangement of electrons under the energy gap is long-range ordered, indicating the existence of interactions between electrons. This interaction is different from Coulomb interaction because it cannot reduce the energy of the system. So the energy gap is formed by the mutual attraction between electrons.[2]

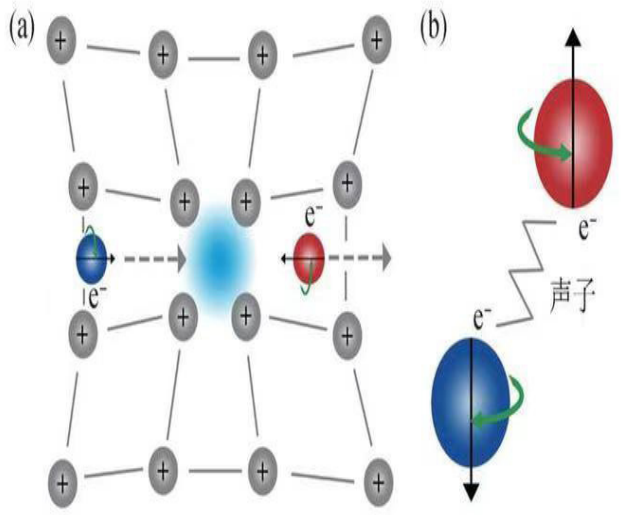

Figure 1 Phonon interaction model

In 1950, Frohlich proposed a model for electron phonon interactions. Phonon is the "Energy quantum of the normal mode of lattice vibration." It is used to describe the harmonic vibration of the lattice and is an important concept in solid-state theory. Assuming that the lattice is arranged neatly, when electrons pass through the lattice, it causes Coulomb interaction between electrons and ion lattice, resulting in lattice distortion. When another electron passes through this distorted lattice, it will be subjected to the effect of a distortion field. Creating the illusion that the first electron attracts the second electron.

$$H_{eff} = \frac{1}{2}\sum_{\substack{q,k_1,k_2 \\ \sigma_1,\sigma_2}} V_{k_1 q} C^{+}_{k_1+q\sigma_1} C^{+}_{k_1-q\sigma_2} C_{k_2\sigma_2} C_{k_1\sigma_1}; V_{k_1 q} = \left|D_q\right|^2 \frac{2\hbar\omega_q}{(E_{k_1+q} - E_{k_1})^2 - (\hbar\omega_q)^2}$$

Frohlich provides the effective interaction potential equation for the longitudinal mode phonon equation of electron exchange, which can be either an attractive potential or a repulsive potential.

When the energy difference before and after the electron undergoes a virtual phonon is less than the phonon energy, the phonon will provide an attractive potential to the electron, shielding the Coulomb effect and pairing the two electrons.

2.3 Cooper pair

The reason why electrical engineering materials exhibit resistance phenomenon is that the electrons inside the material undergo displacement under the action of an electric field and collide with the metal lattice, causing irregular vibrations and generating internal energy macroscopically, which hinders the directional motion of free electrons. The spin quantum number is an integer, and bosons (including photons) that do not follow the Pauli exclusion principle can be infinitely stacked in the same time and space velocity direction, so there will be no energy loss. Two electrons with opposite spin directions (with a spin coefficient of half an integer ± 1/2) combine to form a Cooper pair with a spin coefficient of 0. However, the energy of the Cooper pair is extremely unstable and can only exist stably after entering the Einstein boson condensed state at low temperatures, possessing most of the physical properties of bosons. Therefore, superconductivity and low temperatures are closely related.

2.4 BCS Theory

2.4.1 BCS energy gap equation

According to the Fermi distribution function, in the normal state, electrons exhibit a Fermi sphere distribution, while in the superconducting state, which is the same as in the normal state, electrons do not conduct electricity. Under the dual influence of Coulomb shielding potential field and electron phonon interaction potential field, electrons combine with particles of opposite momentum and spin to form Cooper pairs at a certain temperature. At 0K, Cooper can divide two sets of electron configurations into four situations based on different spin and momentum directions.

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We will linearly superimpose them. It can be obtained that,

$\Psi = c_1\Psi_1 + c_2\Psi_2 + c_3\Psi_3 + c_4\Psi_4$

the total kinetic energy of the system can be calculated as $2\sum_p \epsilon(p)v_p^2$.

$\sum_p$ represents the sum of shell electronic states with a $\hbar\omega_q$ thickness of above and below the Fermi surface.

Considering that the $w_0 = \sum_p 2\epsilon(p)v_p^2 + \sum_{p,p'}(-Vv_pu_p, v_p, u_p)$ potential energy generated by the principle of mutual attraction is - V, the total energy of the system is.

We know that $\frac{\partial w_0}{\partial v_p} = 0$,and order the energy gaps $\Delta = V\left(\sum_p u_p v_p\right)$.

$$2\epsilon(p_1)v_{p_1} - V\left(\sum_p u_p v_p\right)\frac{1-2v_{p_1}^2}{(1-v_{p_1}^2)^{\frac{1}{2}}} = 0; E(p) = \sqrt{\epsilon^2(p)+\Delta^2}$$

Finally, we obtained the BCS energy gap equation[3]

$$\Delta = \frac{V}{2}\sum_p \frac{\Delta}{\sqrt{\epsilon^2(p)+\Delta^2}}$$

2.4.2 Application Status

Superconducting materials research: The BCS theory provides theoretical guidance for the search and design of superconducting materials. For example, when exploring superconducting materials with higher critical temperatures, researchers will screen and optimize the materials based on key factors such as electron-phonon interactions in the BCS theory.

Application of superconducting technology: It has promoted the application of superconducting technology in various fields

Applications in multiple fields, such as magnetic resonance imaging (MRI), maglev trains, high-energy physics experiments, etc. For example, in MRI, superconducting magnets use the zero resistance characteristics of superconductors to generate a strong and stable magnetic field, which provides the basis for obtaining high-quality medical images.

2.4.3 Theoretical advantages

Successfully explaining the phenomenon of superconductivity: explaining it at the microscopic level.

The causes of superconductivity phenomena such as the disappearance of resistance and the Meissner effect in conventional superconductors have given people a deep understanding of the nature of superconductivity. Provide quantitative description: It can quantitatively describe the relationship between some key parameters of superconducting state, such as superconducting energy gap and critical temperature, and the microscopic properties of materials, which provides a theoretical basis for experimental research that can be compared and verified.

Laying a theoretical foundation: It has laid a foundation for the subsequent development and improvement of superconductivity theory, and inspired people to explore more complex problems such as unconventional superconducting materials and high-temperature superconductivity mechanisms.

3. Group theory

3.1 The matrix of force and its eigenvectors

The potential energy V of a crystal is a function of the instantaneous position r (l, k) of an atom. If the displacement u (l, k) of an atom is very small, it can approximate harmonic vibration, and the potential energy of a crystal can be represented by

$$V = V_0 + \frac{1}{2}\sum_{l,k,\alpha}\sum_{l,k,\beta} u_\alpha\begin{pmatrix} l \\ k \end{pmatrix}\Phi_{AB}\begin{pmatrix} l & l' \\ k & k' \end{pmatrix}$$

V_0 represents the potential energy of the crystal in equilibrium state and is a constant.

Among them,

$$\Phi_{AB}\begin{pmatrix} l & l' \\ k & k' \end{pmatrix} = \frac{\partial^2 V}{\partial u_\alpha\begin{pmatrix} l \\ k \end{pmatrix}\partial u_\beta\begin{pmatrix} l' \\ k' \end{pmatrix}}\Big|_{u_\alpha\binom{l}{k}=0, u_\beta\binom{l'}{k'}=0}$$

Is referred to as the force constant.

The force constant is only related to the difference between the lattice vectors R.

Based on the above relationship and combined with knowledge of group representation theory, it can be calculated that:

$$\Phi_{\alpha'\beta'}\begin{pmatrix} L & L' \\ K & K' \end{pmatrix} = \sum_{\alpha,\beta} R_{\alpha\beta}, \Phi_{\alpha\beta}\begin{pmatrix} l & l' \\ k & k' \end{pmatrix}$$

which is the law of transformation of force constant under crystal symmetry operation.

We define m_k as the mass of the kth matrix,

$$D_{\alpha\beta}\begin{pmatrix} l & l' \\ k & k' \end{pmatrix} = \frac{1}{\sqrt{m_k m_{k'}}}\Phi_{\alpha\beta}\begin{pmatrix} l & l' \\ k & k' \end{pmatrix}$$

[4]And the matrix composed of matrix elements is the torque matrix D.

3.2 Dynamics Matrix and Its Eigenvectors

In the field of group theory, studying the harmonic vi-

brations of N atomic lattices is equivalent to solving the eigenvectors of the force matrix. In crystal problems, due to the low dimensionality of crystals, the translational symmetry of crystals can be used to simplify the problem.

$$D_{\alpha\beta}\begin{pmatrix} q \\ kk' \end{pmatrix} \equiv \frac{1}{\sqrt{m_k m_{k'}}} \sum_{\lambda} \Phi_{\alpha\beta}\begin{pmatrix} \lambda \\ kk' \end{pmatrix}$$

3.3 Phonons

We introduce the simplified normal coordinate Q to obtain the crystal vibration equation.

$$\ddot{Q}\begin{pmatrix} q \\ j \end{pmatrix} + \omega^2(q \mid j) Q\begin{pmatrix} q \\ j \end{pmatrix} = 0$$

In order to achieve lattice wave quantization, the real normal coordinates are defined to achieve lattice wave quantization and the corresponding generalized momentum,(η is the dynamic variable describing the harmonic oscillator, which can be obtained using the Lagrange equation.)

$$\eta\begin{pmatrix} q \\ j_p \end{pmatrix} = \frac{1}{2}[Q\begin{pmatrix} q \\ j_p \end{pmatrix} + Q\begin{pmatrix} -q \\ j_p \end{pmatrix}] + \frac{i}{2\omega(q \mid j)}[\dot{Q}\begin{pmatrix} q \\ j_p \end{pmatrix} - \dot{Q}\begin{pmatrix} -q \\ j_p \end{pmatrix}];$$

$$p\begin{pmatrix} q \\ j_p \end{pmatrix} = \dot{\eta}\begin{pmatrix} q \\ j_p \end{pmatrix}$$

The Hamiltonian can be expressed as

$$H = \sum_{q, j_p} \frac{1}{2}[p\begin{pmatrix} q \\ j_p \end{pmatrix}^2 + \omega^2(q \mid j)\eta\begin{pmatrix} q \\ j_p \end{pmatrix}^2]$$

We know the relationship between p and η.

$$p\begin{pmatrix} q \\ j_p \end{pmatrix} = \frac{\hbar}{i}\frac{\partial}{\partial\eta\begin{pmatrix} q \\ j_p \end{pmatrix}}; [p\begin{pmatrix} q \\ j_p \end{pmatrix}]^2 = -\hbar^2 \frac{\partial^2}{\partial\eta\begin{pmatrix} q \\ j_p \end{pmatrix}^2}$$

This way, the Schr ö dinger equation for lattice vibration and its solutions can be written.[5]

$$\{\sum_{q, j_p, \rho} \frac{1}{2}[-\hbar^2 \frac{\partial^2}{\partial\eta\begin{pmatrix} q \\ j_p \end{pmatrix}^2} + \omega^2(q \mid j)\eta\begin{pmatrix} q \\ j_p \end{pmatrix}^2] - E\}\Psi(\{\eta\begin{pmatrix} q \\ j_p \end{pmatrix}\}) = 0$$

ψ is only related to η and is the wave function of a single harmonic oscillator, satisfying the Schr ö dinger equation x of the harmonic oscillator,

$$\frac{1}{2}\{-\hbar^2 \frac{\partial^2}{\partial\eta\begin{pmatrix} q \\ j_p \end{pmatrix}^2} + \omega^2(q \mid j)\eta\begin{pmatrix} q \\ j_p \end{pmatrix}^2 - \epsilon[n(q \mid j_p)]\}\Psi(\{\eta\begin{pmatrix} q \\ j_p \end{pmatrix}\}) = 0$$

Energy ε is quantized, and energy quanta are phonons.[6]

4. The superconducting properties of two types of superconducting materials,

4.1 Yttrium barium copper oxide material

YBCO is a perovskite defect type layered structure containing alternating layers of CuO-CuO_2-CuO_2-CuO, and the CuO_2 layer can exhibit deformation and wrinkles. Yttrium atoms exist in the CuO_2 and CuO_2 layers, while the BaO layer is located between the CuO and CuO_2 layers. When the oxygen atom stoichiometry is less than 7, the structures of these non stoichiometric compounds may vary depending on the specific values, represented by the parameter δ. When δ=1, it is a tetragonal structure, and the CuO layer does not exhibit superconductivity. Slightly increasing the oxygen content will increase the occupancy rate of O. When δ<0.65, Cu-O chains are formed on the b-axis, and the structure becomes orthogonal. The lattice parameters are a=3.82 Å, b=3.89 Å, and c=11.68 Å, respectively. When δ~0.07, the superconductivity is optimal, and only a few of O (1) are empty. There is evidence to suggest that superconductivity occurs in the Cu (2) O layer when other atoms replace Cu and Ba, and Cu (1) O (1) chains are only used for storing charges. However, the superconductivity of compounds formed by replacing yttrium with praseodymium contradicts this. The superconducting length gauge of yttrium barium copper oxygen exhibits anisotropy. Although the coherence length of the a-b plane is as much as six times that of the c-axis, it still appears smaller compared to traditional superconductors such as niobium. This means that its superconducting state is easily affected by interface or cell defects, thus increasing the requirements for instruments used in the production of YBCO, and YBCO is quite sensitive to humid environments. [7]

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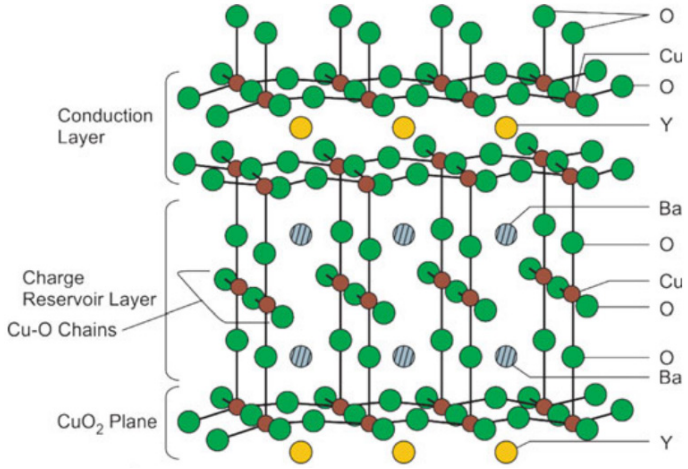

Figure 2 The crystal cell structure of the YBCO material

4.2 Bismuth strontium calcium copper oxide material

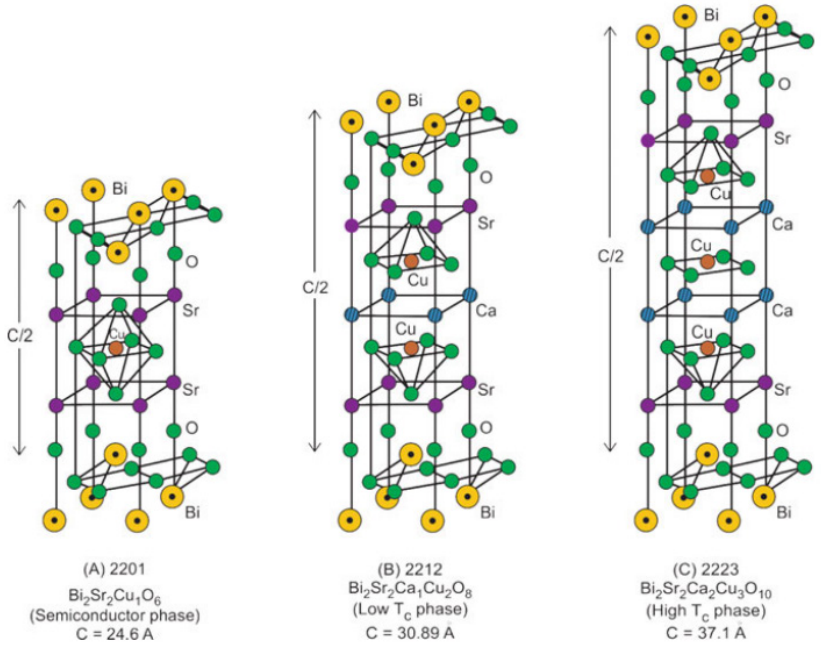

Figure 3 The crystal cell structure of the bismuth strontium copper oxide material

Similarly, bismuth strontium calcium copper oxide materials are also important superconducting materials, which have high critical temperatures, high preparation costs, large anisotropy, small irreversible fields, and a sharp decrease in current carrying capacity under external magnetic fields. The appropriate concentration of doped oxygen atoms in its unit cell structure is crucial for the hollow hole carrier concentration and superconducting properties of copper based superconducting oxides. Therefore, determining the position of doped oxygen atoms and understanding the impact of introducing doped oxygen atoms on the symmetry and electrical and magnetic order parameters of the original crystal is of great significance for understanding the mechanism of superconductivity formation. [8][9]

5. Conclusion

Combining the knowledge of group theory with the analysis of their microstructure, it can be seen that their material electrons and phonons generate interaction forces greater than Coulomb interactions, making it easier to form Cooper pairs at relatively high temperatures. Therefore, they are excellent superconducting materials.

Group theory has many advantages in the study of solid state physics, using the tools of group theory to analyze crystal symmetry, determine crystal classification and structure, study electronic states and band structure, determine band structure, explain physical phenomena, deal with lattice dynamics, analyze lattice vibration mode, study the properties of phonons, etc. Group theory knowledge can simplify complex calculations through matrix representation and concretely represent complex problems. In the future, group theory can help us understand the structure of various materials, speculate the physical properties of various materials, explore the application potential and prospects of various materials, explain more physical phenomena, and promote the development of science and technology.[10]

6. References

[1] SLEIGHT A W. Chemistry of high-temperature superconductors[J]. Science, 1988, 242(4885): 1519-1527.

[2] Chang Haoran, Guo Wei, Huang Lei, Liao Tianfa, Wu Wei, Yang Fujun. Research Progress on High Temperature Superconducting Materials [J], Journal of Hubei University 2023, 1 1000-2375 (2023) 01-0089-08

[3] Zhang Yuheng, Li Yuxi, Superconducting Physics (University of Science and Technology of China Press, 1992)

[4] Xu Wantang, Ka Xinglin, Group Theory and Its Application in Solid Mechanics (Beijing Higher Education Press, 2016).

[5] Micro mass, exploring the relationship between group theory and geometry (insights from physics forum, https://www.physicsforums.com/in-sights/author/micromass, 2016).

[6] E. Khukhro, Group Theory: Algebraic Transformations (Columbia University School of Mathematics and Physics, 2017).

[7] R.G. Sharma Superconductivity --Basics and Applications Magnets(Springer Series in Materials Science 214)

[8] The latest progress of bismuth strontium calcium copper oxygen superconducting oxide in Tsinghua AFM [J]. Science and Technology Workers' Home. December 8, 2019. https://doi.org/10.1002/adfm.201903843

[9] ZOLLER P, GLASER J, EHMANN A, et al. Superconductivity and processing of single Bi-O layered cuprates in the (Bi, Pb) -Sr-(Ca, Y) -Cu-O system[J]. Zeitschrift für Physik B Condensed Matter, 1995, 96(4): 505-509.

[10] P. Tixador, Superconducting magnetic energy storage: status and perspective, in IEEE/CSCand ESAS European Superconductivity News Forum, vol. 3, Jan 2008.www.ewh.ieee.org/europe/ newforum/pdf/CR5_final3_012008.pdf