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STUDY ON THE EFFECT OF THE COULOMB INTERACTION ON SUPERCONDUCTIVITY AND ITS APPLICATION TO N-TYPE SEMICONDUCTING $SrTiO_3$

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By solving the gap equation from the first principles, we study the effect of the plasmon on superconductivity and investigate the mechanism of superconductivity in n-type semiconducting $SrTiO_3$. The observed transition temperature as a function of the carrier density and the applied stress is reproduced well, when we take account of the plasmon and the polar optic phonon which relates to the stress-induced ferroelectric transition.

I. Introduction

The Coulomb interaction between electrons has not usually been considered to give any contributions to the formation of the Cooper pair. Thus this interaction has been treated much more simply than the phonon-mediated interaction. In the conventional method to calculate the transition temperature T_c of metallic superconductors[1], its effect has been estimated by one adjustable parameter μ^* called the Coulomb pseudo-potential. However, the idea of μ^* is appropriate only when the Debye energy ω_D is much smaller than the Fermi energy ε_F. In low-carrier-density systems such as degenerate semiconductors having ε_F of the order of ω_D, the effect of the Coulomb interaction should be treated more seriously.

In the present study, we employ a method of calculating T_c in which the value corresponding to μ^* is determined from the first principles. For this purpose, a cutoff energy, which is usually taken of the order of ω_D, is not introduced in the gap equation. With the use of this method, we study the effect of the plasmon on superconductivity and find that this effect becomes so large in low-carrier-density systems that the value corresponding to μ^* becomes negative. This method is then applied to n-type semiconducting $SrTiO_3$ in order to explain the mechanism of superconductivity observed in this material[2,3].

II. Gap Equation

At T_c, the equation for the gap function $\Delta(\omega)$ is given in the weak-coupling approximation as

$$\Delta(\omega) = -\int_{-\varepsilon_F}^{\infty} \frac{d\omega'}{2\omega'} \tanh \frac{\omega'}{2T_c} K(\omega,\omega')\Delta(\omega'), \qquad (1)$$

with the kernel $K(\omega,\omega')$, defined by

$$K(\omega,\omega') = \frac{m^*}{4\pi^2 p}\int_{|p-p'|}^{p+p'} q\,dq \int_0^{\infty} \frac{2}{\pi} d\Omega \frac{|\omega|+|\omega'|}{\Omega^2+(|\omega|+|\omega'|)^2} V^R(q,i\Omega), \qquad (2)$$

where m^* is the effective mass, p and p' are, respectively, related to ω and ω' through the relations of $p=\sqrt{2m^*(\omega+\varepsilon_F)}$ and $p'=\sqrt{2m^*(\omega'+\varepsilon_F)}$, and $V^R(q,i\Omega)$ is the effective electron-electron interaction in the retarded form. Equation (1) with eq.(2) was first derived by Kirznits et al.[4] and the numerical method to solve this equation was presented in [5].

Analytic solution of eq. (1) can be given easily, if $K(\omega,\omega')$ is assumed to be

$$K(\omega,\omega') = K(0,0) + \{F(\omega)+F(\omega')\}\,\theta(\varepsilon_F-|\omega|)\,\theta(\varepsilon_F-|\omega'|), \tag{3}$$

where $\theta(\omega)$ is the Heaviside function and $F(\omega)$ is free from all the restrictions except that $F(0)=0$. In this form of the kernel, the condition to appear superconductivity is obtained as

$$\int_{-\varepsilon_F}^{\varepsilon_F} \frac{d\omega}{2|\omega|} F^2(\omega) > K(0,0). \tag{4}$$

III. Role of the Plasmon

When we consider an electron-gas system, V^R in eq. (2) is given by the Coulomb interaction $4\pi e^2/\varepsilon_\infty q^2$ screened by the electrons themselves. Then $K(0,0)$ becomes so-called μ-parameter. The plasmon contributes to the change of $K(\omega,\omega')$ even near the Fermi surface and $F(\omega)$ in eq. (3) is given for small $|\omega|$ as

$$F(\omega) \approx 0.176\sqrt{r_s}\,|\omega/\varepsilon_F|\,\ln 4|\varepsilon_F/\omega|, \tag{5}$$

where r_s parameter is defined as usual by $r_s = m^* e^2/\varepsilon_\infty \times (3/4\pi n)^{1/3}$ with the carrier density n. The coefficient in eq. (5) is determined by the f-sum rule, so that it is independent of the approximation used in the calculation of V^R. The contribution of the plasmon increases as r_s increases, while μ-parameter does not change so much for large r_s. Therefore we can predict with the use of the inequality (4) that superconductivity appears even in an electron-gas system.

The result of T_c given by the numerical solution of eq. (1) is shown in Fig. (1) as a function of n. In an electron-gas system, T_c and n are, respectively, normalized by the effective Rydberg m^*/ε_∞^2 and the effective Bohr radius cubed $(m^*/\varepsilon_\infty)^3$, where m^* is in the unit of the mass of a free electron. Irrespective of the approximation to V^R, superconductivity appears in rather low-density systems.

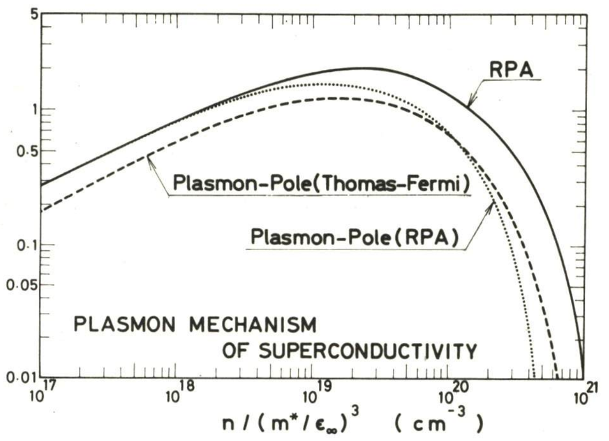

Fig.1 Superconducting transition temperature T_c as a function of n in an electron-gas system: Solid, broken and dotted lines correspond to the results in the RPA, the plasmon-pole approximation with the Thomas-Fermi static interaction, and that with the static RPA interaction, respectively

The behavior of the curve of T_c can be explained as follows. When ω is of the order of the plasmon energy ω_p, $V^R(q,\omega)$ has the form for small q as

$$V^R(q,\omega) \approx \frac{4\pi e^2}{\varepsilon_\infty q^2}\cdot\frac{1}{1-\omega_p^2/\omega^2}. \tag{6}$$

Thus, contrary to the case in which acoustic phonons are exchanged, the effective interaction $V^*(r)$ for the pair which exchanges the plasmon becomes negative for large r as

$$V^*(r) \approx -e^2/\varepsilon^* r, \tag{7}$$

where r is the mutual distance of the pair and ε^* is the effective

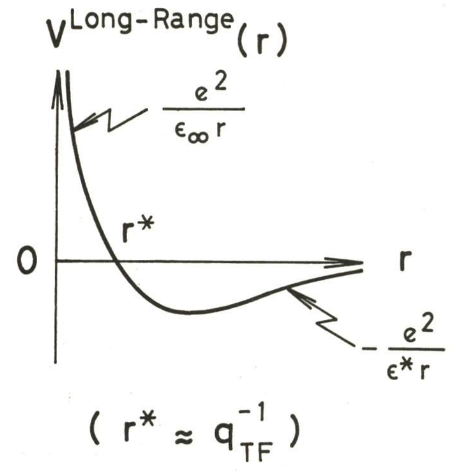

Fig.2 Effective potential for a Cooper pair formed by the exchange of the plasmon

strength of the attractive potential induced by the virtual exchange of the plasmon, given tentatively by $\varepsilon^* = \omega_p^2/\varepsilon_F^2$. On the other hand, when r is small, the Coulomb repulsion is most important and $V^*(r)$ can be taken as

$$V^*(r) \approx e^2/\varepsilon_\infty r. \tag{8}$$

From these two asymptotic behaviors of $V^*(r)$, the effective interaction can be simulated by $V^{\text{Long-Range}}(r)$ in Fig. (2). The value r^* in the figure connects these two asymptotic forms and can be taken to the Thomas-Fermi screening length q_{TF}^{-1}. Under this potential $V^{\text{Long-Range}}$, T_c, i.e., the binding energy of the pair, becomes proportional to $(\varepsilon_\infty/\varepsilon^*)\times\exp(-r^{*2}p_F^2)$. The first factor, $\varepsilon_\infty/\varepsilon^*$, comes from the attractive part and increases with the increase of n. The second factor, $\exp(-r^{*2}p_F^2)$, arises from the repulsive part and decreases with n. These two opposite behaviors make the maximum in the curve of T_c.

The preceding discussion is done in the weak-coupling approximation. But this is not always valid. In particular, there remain problems when n is small. Thus further study should be done on the problem whether an electron-gas system becomes superconducting or not.

IV. Application to $SrTiO_3$

Several people have already discussed the mechanism of superconductivity in $SrTiO_3$. All of them except Koonce et al.[2] used the idea of μ^*, though it is not good because ω_D/ε_F is of the order of unity in this case. Futher, Koonce et al. used the Cohen's theory[6], but the Cohen's theory cannot take account of the effect of the plasmon properly.[7] Thus we study this material here including the effect of the plasmon.

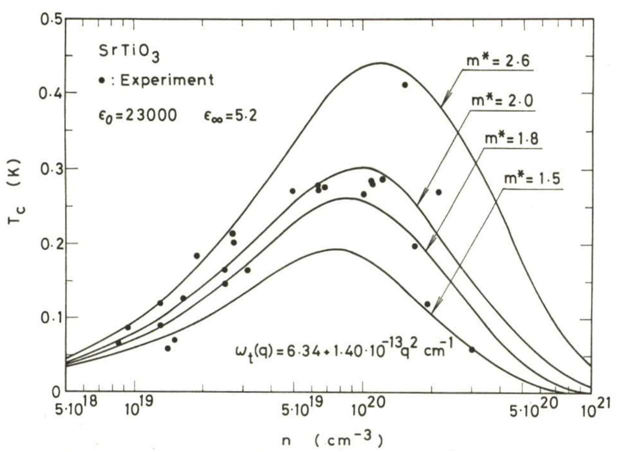

Fig.3 Calculated T_c as a function of n for several values of m^* in the plasmon-ferroelectric soft optic phonon mechanism of superconductivity

The effective interaction to be considered is given by

$$V^R(q,\omega) = 4\pi e^2/q^2\varepsilon^R(q,\omega), \tag{9}$$

with

$$\varepsilon^R(q,\omega) = \varepsilon_\infty + \frac{4\pi e^2}{q^2}\Pi^R(q,\omega) + [\varepsilon_0(q)-\varepsilon_\infty]\frac{\omega_t^2(q)}{\omega_t^2(q)-\omega^2-i0^+} \tag{10}$$

and

$$\varepsilon_0(q) = \varepsilon_0\,\omega_t^2(0)/\omega_t^2(q), \tag{11}$$

where $\Pi^R(q,\omega)$ is the electronic polarization which is calculated in the RPA, $\omega_t(q)$ is the energy of the transverse ferroelectric optic phonon, and ε_∞ and ε_0 are, respectively, the optic and the static dielectric constants.

Taking the values ε_0=23000, ε_∞=5.2 and $\omega_t(q)=6.34+1.40\times10^{-13}q^2$ cm^{-1} determined from experiments, T_c is calculated as a function of n from the first principles for several values of m*. Figure (3) shows the result with experimental points[2]. The experiment can be reproduced well for m* in the range from 1.5 to 2.0 in which region the experimental value of m* lies. The behavior of T_c is almost the same as appeared in Fig.(1). This arises from the fact that both the plasmon and the ferroelectric soft optic phonon produce the long-range attractive potential.

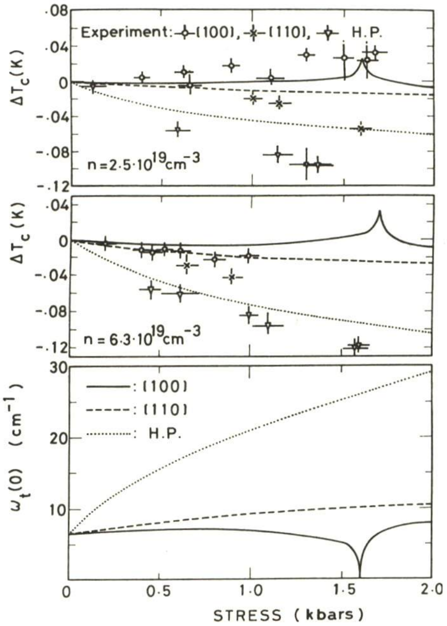

Fig.4 Calculated stress effects on T_c: Cases of the hydrostatic pressure, the uniaxial stresses along the [100] and the [110] directions are indicated by H.P., [100], and [110], respectively

The stress effect on T_c is also investigated by changing $\omega_t(0)$ with the stress. The calculated results of the change of T_c are shown in Fig.(4) in the bottom of which the experimental data on $\omega_t(0)$ are given. The value of m* is taken to be 1.8. The experimental behavior of T_c, i.e., T_c decreases with the hydrostatic pressures (H.P.), while T_c sometimes increases in the [100] uniaxial stresses, is explained well in the present mechanism.

Other modes like the acoustic phonon are also included in V^R, but their effects are small. The weak-coupling approximation does not seem to produce a big problem in this system, because ε_0 is very large and makes the effective interaction weak. In this way, the superconductivity in $SrTiO_3$ may be concluded to be due to the plasmon and the ferroelectric soft optic phonon.

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