Superconductivity as a consequence of an anomalous nonlinear polarizability of electrons with an extremum surface in the dispersion law

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For a semiconductor which has a surface or line (or loop) of extrema there exists an interval of doping levels in which the correlation energy exceeds the kinetic energy, even in the case of a weak interaction. In this case, superconductivity would arise as the result of an electron-electron attraction stemming from the quadratic nonlinear polarizability of the same electrons.

The superconductors of the high-temperature group based on copper oxide exhibit many anomalous properties in their nonsuperconducting phase: proximity to a metal-semiconductor phase transition, proximity to an antiferromagnetic phase transition, etc. One direction in explaining these anomalies and the high critical superconducting temperature T_c is based on the suggestion that because of the strong Coulomb repulsion (U) of two electrons at a common center in comparison with the width (W) of the allowed band it would be more appropriate to speak in terms of localized electrons,

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rather than Bloch electrons. Unfortunately, even in this approximation, $U \gg W$ (see Refs. 1 and 2, for example), we do not yet have a rigorous, systematic description of superconductivity. Furthermore, the small values which have been observed for the dielectric gap, E_g and the values found for W from band calculations (these values are not small) indicate that if a localization does occur, then it must be described in the approximation $U \approx W$. Whether the primary reason for the attractiveness of this direction—superconductivity exclusively as a result of Coulomb correlations—is retained in the case $U \approx W$ is an open question. In our opinion, a convincing answer to this question would be the proof that a superconductivity due to Coulomb correlations is possible in the opposite case, $U \ll W$. We offer such a proof in the present letter.

We consider the situation in which the normal metallic state is characterized by the presence of congruent parts of the Fermi surface ("nesting"). As W is reduced, and we go from the approximation of nearly free electrons ($U \ll W$) to the case of localization at the atomic scale ($U \gg W$), we have a wide interval in the parameter W/U in which the overlap of the wave functions at nearest neighbors is substantially greater than the overlap with next-nearest neighbors. In this case, with a half-filled band (one electron per unit cell), the nesting condition can be satisfied easily[3] even in the three-dimensional ($3D$) case and especially in the two-dimensional ($2D$) case. The interrelationship between the dielectric and magnetic correlations, on the one hand, and the superconductivity, on the other, can be described asymptotically exactly[4,5] (see also Ref. 6) in such systems (in contrast with the case $U \gg W$). Here there can be a dielectric behavior even in the absence of a corresponding charge long-range order (charge density wave) or spin long-range order (spin density wave) by virtue of the macroscopic (30–300 Å) short-range order.[7] As in the approximation $U \gg W$, a superconductivity is possible only to the extent that there is a doping with a density n (of electrons or holes), and T_c goes through a maximum as a function of n, in agreement with experiment.

In this case the large value of T_c stems from the square-root singularity $1/\sqrt{E}$ in the state density near the extrema of the valence and conduction bands of the semiconductor phase, which are separated by a gap E_g or a pseudogap[5] (in the absence of a long-range order). It has been suggested that an electron-electron attraction mechanism (e.g., a phonon mechanism) be specified for a superconducting gap which has no zeros at the Fermi surface.

The state-density singularity which we just mentioned ($1/\sqrt{E}$), which leads to an increase in T_c, by a factor of 20, for example, at a coupling constant $\lambda \approx 1$ (Ref. 5), occurs because the extrema of the bands in the semiconducting phase form a surface ($3D$) or line ($2D$) in momentum space with a typical dimension p_0 (which is on the order of a reciprocal-lattice vector). Such a state is thus the limiting case of a multivalley semiconductor with an infinite number of valleys, ν. With increasing carrier (e.g., hole) density n, the growth of the kinetic energy $\epsilon_F = p_F^2/2m^*$ slows down, by virtue of the relation $p_F \sim (n/\nu)^{1/3}$. There is accordingly an interval in n in which we have $p_F a_{FB}^* \gg 1$, i.e., in which the random phase approximation holds, but the correlation energy E_{corr} is greater than the kinetic energy[8] (a_B^* is the first Bohr radius in the semiconductor). In the case in which we are interested we would have

$p_F = b_3\hbar^3 n p_0^{-2} \equiv N_3^{-1} n(3D)$, $p_F = b_2\hbar^2 cn p_0^{-1} \equiv N_2^{-1} n(2D)$ (the coefficients $b_3 \sim 10$ and $b_2 \approx 5$ depend on the geometry of the surface or line, respectively, of extrema), $a_B^* = \hbar\epsilon_\infty^*/e^2 m^*, m^* = E_g/v_0^2$, and $\epsilon_\infty^* \sim E_g^{-1}$, where v_0 is the Fermi velocity in the metallic phase, and c is the distance between layers (the overlap of the wave functions between layers is being ignored).

Under the condition $1 \ll p_F a_B^* \ll (n a_B^{*3})^{1/4}$, which we see from the expression for p_F corresponds to

$$N_{2,3}\, a_B^{*2} \ll n a_B^{*3} \ll (N_{2,3}\, a_B^{*2})^{4/3} \tag{1}$$

the correlation energy is dominated, as in Ref. 8, by momenta $q \sim n^{1/4}$ and frequencies $\omega \sim n^{1/2}$. The total energy per electron reaches its minimum value at the density $n_{\min} a_B^{*3} = (N_{2,3} a_B^{*2})^{8/7}$; this minimum value is

$$E_{min} = -\,\mathrm{Ry}\left(\frac{a_B^* p_0}{\hbar}\right)^{4/7} (3D), \qquad E_{min} = -\,\mathrm{Ry}\left(\frac{a_B^{*2} p_0}{c\hbar}\right)^{2/7} (2D)\,, \tag{2}$$

where $\mathrm{Ry} = e^4 m^*/2\hbar^2\epsilon_\infty^*$ is the binding energy of an exciton. The energy $E_{\min}$ given by (2) is substantially greater than the exciton binding energy.

Under conditions (1), because of the same factor which makes the correlation energy important, the following series of diagrams[9] (Fig. 1) for the vertex function $\Gamma(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q})$ attracts attention. A wavy line here corresponds to a screened Coulomb interaction $V/(1 - V\Pi_0)$. Diagrams a and b,

$$\gamma = -\frac{1}{2\pi^2}\int \frac{d^3 q\, d\omega}{(2\pi)^4}\left[\frac{V(\mathbf{q})}{1 - V\Pi_0(\mathbf{q}, \omega)}\right]^2 G(\mathbf{p}_1 + \mathbf{q})\, G(\mathbf{p}_2 - \mathbf{q}), \tag{3}$$

are dominated by the regions $q \sim n^{1/4} \gg p_F$ and $\omega \sim n^{1/2} \gg \epsilon_F$, and for $\mathbf{p}_1$ and $\mathbf{p}_2$ on the order of p_F the value of γ does not depend on $\mathbf{p}_1$ or $\mathbf{p}_2$ and has the value[9] $-A_\gamma n^{-3/4}$. In other words. this value corresponds to an electron-electron attraction. We then find the following expression for the quantity Γ, which appears as a "seed" initial diagram in the equation for T_c:

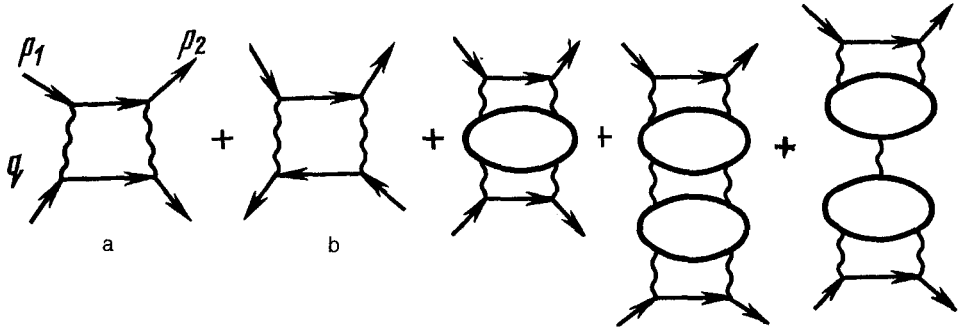

FIG. 1.

$$\Gamma(\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}) = (V + \gamma)[1 - \Pi_0(\mathbf{q}, \omega)(V + \gamma)]^{-1}. \quad (4)$$

At $n > n_{cr} \approx n_{min}$, the denominator in (4) is on the order of unity. In this model, the equations for T_c are dominated by $q \sim n^{1/4} \gg p_F$, instead of $q \sim p_F$, as in the model of Ref. 10. Under the assumption of a strong frequency dispersion of the dielectric constant, $\epsilon^*(\omega)$, in the region of phonon frequencies $\omega_0[\epsilon^*(0) \equiv \epsilon_0^* \gg \epsilon^*(\omega \gg \omega_0) \equiv \epsilon_\infty^*]$, as is typical of copper-oxide superconductors, the Coulomb interaction is governed by the value of ϵ_0^*, and γ is governed by ϵ_∞^*. The reason for the latter circumstance is that in the expression for γ the zeroth transferred frequency is given as the difference between two frequencies, each of which is proportional to $n^{1/2}$, i.e., to the plasma frequency. As a result, under the conditions

$$\epsilon_0^* > \frac{\epsilon_\infty^*}{b_3^{2/7}} (a_B^* p_0)^{4/7} (3D), \qquad \epsilon_0^* > \epsilon_\infty^* \left(\frac{a_B^{*2} p_0}{b_2 c} \right)^{2/7} (2D) \quad (5)$$

the electron-electron attraction due to the nonlinear (quadratic) polarizability will outweigh the direct Coulomb repulsion, which is characterized by a positive dielectric constant ϵ_0^*. The effective coupling constants

$$\lambda_{3D} \equiv \frac{m_0 p_0}{\hbar} |\gamma| = \frac{e^2}{\hbar v_0 \epsilon_\infty^*} \left[\frac{a_B^{*2} p_0^2}{\hbar^2 (n a_B^{*3})^{3/4}} \right],$$
$$\lambda_{2D} \equiv \frac{m_0}{c} |\gamma| = \frac{e^2}{\hbar v_0 \epsilon_\infty^*} \left[\frac{a_B^* p_0}{\hbar c (n a_B^{*3})^{3/4}} \right], \quad (6)$$

must be substituted into the corresponding expressions[4-6] for T_c if this correlation attraction mechanism is dominant. Everywhere above we have assumed $E_g \gg \epsilon_F$ and $E_g \gg \tilde{\omega} \sim n^{1/2}$. In the case $\tilde{\omega} > E_g \gg \epsilon_F$, on the other hand, we need to replace m^* by $m_0 = p_0/v_0$ in the region of electron energies where the characteristic momenta are $q \sim n^{1/4}$. This increase in the state density at energies on the order of $\tilde{\omega}$ leads to an increase in the value of γ and thus that of λ by a factor of $m_0/m^* \gg 1$.

One might hope that the superconductivity mechanism discussed under conditions (1) would remain qualitatively in force at $n a_B^{*3} \sim 1$.

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