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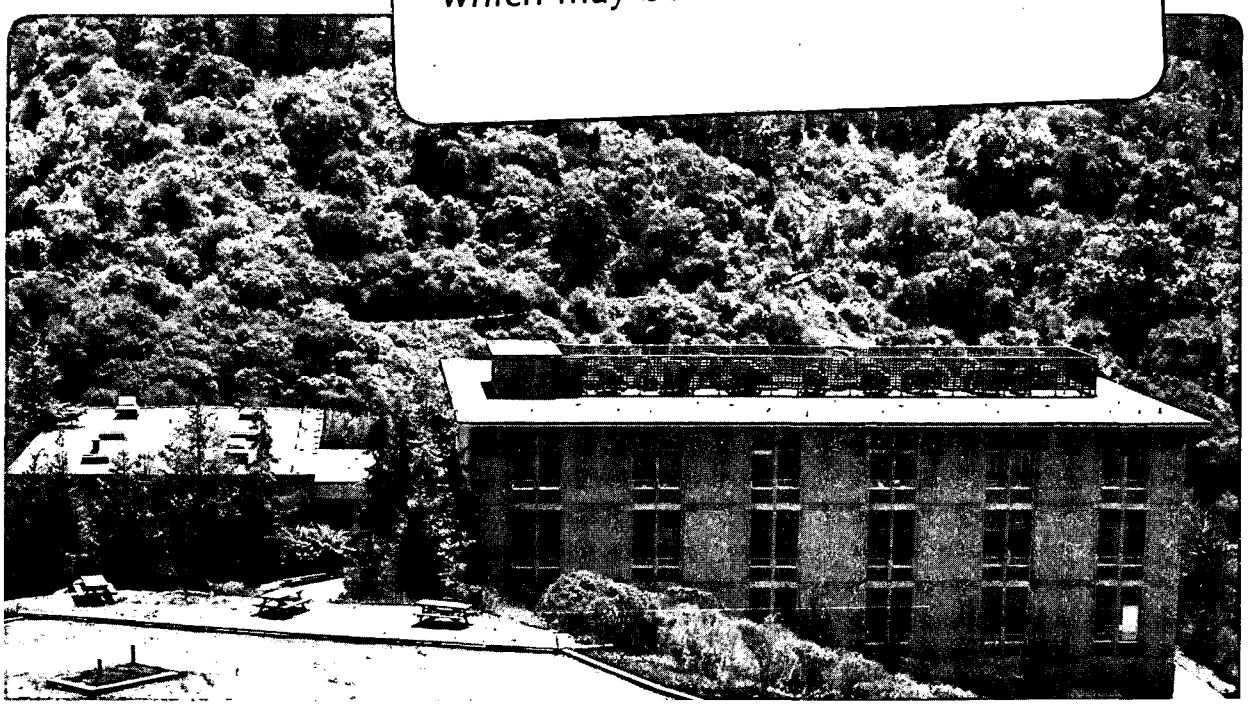

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PHONON-PLASMON MECHANISM OF HIGH T_c SUPERCONDUCTIVITY

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The observed high superconducting transition temperatures are caused, in our view, by the coexistence of strong electron-phonon coupling and the plasmon mechanism. A generalized Eliashberg equation describing the effects of phonons and plasmons on the pairing is presented. The structure of the plasmon bands in conducting, highly anisotropic layered materials are studied.

Introduction. The new high T_c materials [1,3] display BCS-type superconductivity. This implies: 1) pairing due to exchange of excitations of some intermediate field; 2) the presence of an energy gap. According to the usual BCS theory, which describes with great success the properties of hundreds of conventional superconductors, the superconducting state is due to an effective electron-electron interaction via exchange of virtual phonons. As regards the new high T_c materials, we think that in addition to phonons, a very important role is played by plasmons. As is known, plasmons arise from the collective motion of the carrier subsystem, whereas phonons describe the quantized excitations of the ionic lattice.

The role of plasmons in high T_c superconductivity has been pointed out and described in our papers [4,5]. Later, various aspects of the electron-plasmon interaction and plasmon mechanisms were discussed in [6].

The question for the origin of high T_c by virtual exchange of some intermediate field may be further broken down into two distinct parts of each of which has to be met to be taken seriously:

(1) The physical demonstration of the existence of the particular excitation invoked for the mechanism.

(2) The coupling of the carriers to be paired to this excitation.

For phonons and plasmons the answer to (1) is positive. Quasi-2D plasmons have been observed experimentally in [7] (infrared spectroscopy electron

losses). For excitons there seems to be no evidence for a strong optical excitation up to an upper limit of 5-6 eV. For magnetic excitations and magnetic (anti-ferromagnetic) ordering there are experimental observations with Neel temperatures of several hundred degrees K in both undoped and slightly doped La_2CuO_4 and Y $Ba_2CU_3O_{6+\delta}$ [8] in the insulating phase. The Neel temperatures observed decreased with increased doping or increasing δ suggesting that the anti-ferromagnetic and conducting states of the system are unable to coexist. On the other hand, a detailed polarized neutron scattering result [9] on the superconducting $YBa_2Cu_3O_7$ showed no evidence of magnetic excitations in the expected energy region probed by inelastic neutron scattering.

First of all, we would like to stress that the high T_c in the new materials is due not to the plasmon mechanism by itself, but to its coexistence with strong electron-phonon coupling. On the other hand, there is experimental evidence that the electron-phonon interaction is very important, but it is not sufficient to lead to the observed high transition temperatures.

Speaking of exchange by phonons and plasmons, one should note that these are not hypothetical, but real excitations. At the same time, the high anisotropy of the new oxides, caused by the presence of layer and chain structures, makes the plasmon mechanism very favorable. The behavior of plasmons in quasi-low-dimensional materials, their dispersion relations, etc., differ in a striking way from those in the usual 3D systems. The interaction of an electron with the rest of the Fermi sea is not only responsible for the usual screening, but, in addition, it contains a dynamic part. This dynamic part corresponds to the collective motion of electrons with respect to the lattice or to the relative motion of two groups of carriers in a system with two energy bands. Plasmons are the quasi-particles describing such collective motion, and, in this case, they are similar to phonons which are the quasi-particles describing the collective excitations of the lattice.

Interaction. Consider a highly anisotropic system with a layered structure. The z-axis is chosen to be perpendicular to the layers. Our approach assumes the applicability of the Fermi liquid description of the system. Such an approach has been used by S. Wolf and one of the other authors [10] in order to evaluate the major parameters of the oxides. A recent positron annihilation data [11], indeed, have resulted in the obtaining the Fermi surface of Y-Ba-Cu-O system, in agreeing with [10].

The self-energy part $\Delta(\vec{K}, P_z, \omega_n)$ ($\vec{K}$ is a 2D momentum, $\omega_n=(2n+1)\pi T$) is described by the equation

$$\Delta(\vec{\varkappa}, P_z, \omega_n) Z = T\sum_{\omega_n'} \int d\vec{\varkappa}\, dp_z' \times$$

$$\times \Gamma(\vec{\varkappa}-\vec{\varkappa}'; P_z; P_z'; \omega_n - \omega_n') F^+(\vec{\varkappa}', P_z', \omega_n'). \qquad (1)$$

Here F^+ is an anomalous Green function, Z is the renormalization functions, and I is the total vertex describing the effective electron-electron interaction.

The total vertex can be written in the form $\Gamma = \Gamma_{ph} + \Gamma_{ph'}$. Γ_{ph} describes the electron-phonon interaction: $\Gamma_{ph} = g^2 D$, where D is the phonon Green's function and g the electron-phonon coupling constant. Note that the region of the crossing of the optical phonon and plasmon branches should be considered separately, then it is necessary to take into account the hydridization of the branches.

Plasmons in Anisotropic Metals. The pure 2D dispersion relation was obtained in [10] and analyzed in detail by us in [4,5].

The existence of a low-lying plasmon branch, which does not have an energy gap at q=0, is a major difference between 2D and 3D plasmons. It is important that this branch exists even for a single energy band. Appearance of the additional "demon" branch caused by overlap at partially-filled bands.

2D dispersion relation can be obtained in the random phase approximation (RPA. As is known, RPA can be modified by introducing the special function G(q) [13]: $G(q)=A[1-e^{-B(q/P_f)^2}]$, where A and B depend on r_s. This modification leads to a change in the dispersion relation. As a result, we obtain the same plasma branch $\omega \sim q^{1/2}_{q\to 0}$, but with a modified coefficient of the dispersion relation.

Interlayer interaction leads to a noticeable modification of the pure 2D dispersion relation, namely to the formation of plasmon bands. Nevertheless, anistropy results in a picture which differs in a striking way from the isotropic 3D case. In addition, the maxima of the plasmon density of states are shifted towards the boundaries of the plasmon branches, which enhances the electron-plasmon coupling considerably. In our view, it is the layered nature of the superconducting cuprates which confines the collective motion of the electrons predominantly to the planes and leads to the unusual features of its plasmon spectra.

Two factors due to interlayer interactions affect the plasmon dispersion relation. Firstly, the interlayer Coulomb interaction plays an important role. Secondly, one should consider interlayers transitions of the electrons. (The importance of this factor increases with decreasing interlayer distance.) The new high T_c materials are characterized by high anistropy of the normal conductivity [12]. This means that the major modification of the dispersion relation comes from the first factor, that is, from the Coulomb interaction. The Fermi surface of a layered structure has a cylindrical shape [13] with the electron dispersion relation $\varepsilon(\vec{\mathcal{K}})$, where $\mathcal{K}$ is the 2D quasi-momentum. A small deviation from the cylindrical shape is a manifestation of interlayer transitions.

Layered crystals are characterized by a plasmon band $\Omega = f(\kappa, k_z)$, where $\vec{\kappa}$, k_z are wave vectors in the planes and perpendicular to them. The z-axis is chosen to be perpendicular to the layers.

The values of Ω are restricted to lie between the upper and lower branches. These branches correspond to $k_z=0$ and $k_z=\pi/c$ for the uppermost and the lowest branches, respectively. In addition, we note that these boundary modes correspond to in-phase motion of electron on different planes ($k_z=0$) and out-of-phase motion ($k_z=\pi/c$) on adjacent planes. Note that the layer spacing c is equal to half the lattice constant c_o for $La_{2-x}Sr_xCuO_4$.

In Fig. 1, we show the dispersion relations for the layered electron gas in a cylindrically symmetric system -- the excitations are both electron-hole pairs and the various plasmon branches for the in-plane wave vector, k, and the wave vector perpendicular to the conducting sheets, Pz

The upper branch corresponds to three-dimensional behavior, and the dependence of $\Omega(k, 0)$ is similar to the behavior of the usual three-dimensional sample. On the other hand, the behavior of the lowest branch $\Omega(k,\pi/c)$ is entirely different. It is important to note that in the limit $k_z \gg 1/c$, the interlayer interaction does not play an important role, and we are dealing with a two-dimensional dispersion relation ω k. There is a crossover from 3D to 2D behavior in the region $k_z \sim 1/c$. This crossover

corresponds to a maximum in the density of states. This can be seen by considering the dependence of the plasmon frequency Ω on one less variable and hence, the derivative with respect to this variable goes to zero. This leads to an effective increase in the density of states in this region.

Hence, interlayer interaction leads to the formation of a highly anisotropic plasmon band $\Omega(k,k_z)$. A very important feature of this band is the nonuniform distribution of the density of states.

One can show, [5] that the plasmon density of states has two peaked regions [ ]. The sharp increase of the density of states near the lower boundary is particularly important for the superconducting state.

Plasmon-Optical Phonon Hybridization. In this section, we want to draw attention to the potential hybridization of electronic charge density oscillations with ionic charge motion such as polar modes [ ]. This case corresponds to the crossing of the plasmon and optical phonon branches. Then the total vertex cannot be written as a sum (2), and this means that it is impossible to separate the excitations.

As a result of this hybridization, the two branches acquire characteristics of each other as in standard polariton theory. The modes do not cross, but are split off from each other by an amount dependent on the strength of the coupling. This coupling in the lowest approximation is proportional to the product $\sim \rho_{pl}\rho_{ph}$ where $\rho_i=\lambda_i[1+\lambda_{ph}+\lambda_{ph}]^{-1}$, i=pl,ph. A large value of λ_{ph} may result in a noticeable splitting. The lower branch strongly disperses in the intermediate frequency region ($100\ cm^{-1}<\omega<1000\ cm^{-1}$). As a consequence, the plasmon density of states behaves similarly to the usually phonon density of states.

The function $g_{pl}(\omega)$ is, therefore, characterized by a strong peak in the intermediate frequency range. This peak has a structure similar to the usually phonon peak and can be determined by tunneling spectroscopy. Because of the mixing of electronic and ionic degrees of freedom, it seems plausible that optical measurements in this frequency region will be enhanced over purely ionic oscillator strength. There is recent experimental evidence for very strong absorption in the phonon region in both the La-Ba-Cu-O and Y-Ba-Cu-O systems [14].

Superconducting State: Coexistence of the Phonon and Plasmon Mechanisms. As was noted in the Introduction, our approach is based on the concept of coexistence of the phonon and plasmon mechanisms. At present, this concept is receiving various experimental support.

Experimental data on thermal conductivity [15], heat capacity [16], sound attenuation [17], etc., show that the electron-phonon coupling plays an important role.

The increase of the thermal conductivity $\mathfrak{X}(T)$ at temperatures $T<T_c$ observed in [15] means (see e.g., [18]) that the phonons make a major contribution to the total thermal flow, and the electron-phonon interaction (EPI) is a main relaxation mechanism. EPI was analyzed in [16] with the use of the heat capacity data. The method [16] is based on the dependence of the Sommerfeld's constant on temperature (see [19]). As a result, the value was obtained.

Strong electron-phonon coupling is very important for high T_c but, nevertheless, it is not sufficient and there is a need for an additional mechanism. Indeed, let us consider the question: how large a value of λ_{ph} in La-Sr-Cu-O is required in order to provide $T_c \simeq 40K$. In order to answer this, it is convenient to use the expression for T_c obtained in [20].

$$T_c = \frac{0.25\tilde{\Omega}}{[e^{2/\lambda_{eff}}-1]^{1/2}} . \qquad (3)$$

Here $\tilde{\Omega} = \langle\Omega^2\rangle^{1/2}, \langle\Omega^2\rangle = \int d\Omega\, \alpha^2(\Omega)F(\Omega)\Omega$, $F(\Omega)$ is the phonon density of states, $\alpha^2(\Omega)$ describes the electron-phonon interactions; $\lambda_{eff} = (\lambda - \mu^*)(1 + 2\mu^* + \mu^*\lambda + \mu^*\lambda t(\lambda))^{-1}$ the function $t(\lambda)$ is defined in [20]. Equation (3) was obtained directly from the Eliashberg equation and is valid for any value of λ_{ph} (for more detailed analysis and limiting cases, see [20].

Let us apply Eq. (3) to the La-Sr-Cu-O system in order to estimate the value of λ_{ph}. According to data obtained by neutron inelastic spectroscopy [21], the phonon density of states $F(\Omega)$ in the $La_{1.8}Sr_{0.2}CuO_4$ system exhibits two sharpe peaks at $\Omega_1 \simeq 100K$ and $\Omega_2 \simeq 200K$. The function $\alpha^2(\Omega)$ can be determined by the tunneling spectroscopy technique (these measurements have not yet been carried out) but usually $\alpha^2(\Omega)$ is a relatively smooth function. As a result, it is reasonable to put $\tilde{\Omega} \simeq 150K$. Assuming that $\mu^* \simeq 0.1$ (larger values of μ^* lead to an increase of λ_{ph}, see below), we obtain from Eq. ( ): $\lambda_{ph} \simeq 5$. This means that the electron-phonon interaction can account for the high $T_c \simeq 40K$ in La-Sr-Cu-O compound, but this requires very strong coupling.

The value of λ_{ph} for different materials can be measured with the use of tunneling spectrocopy, but the data are unavailable at present. However, the necessary information can be obtained from another set of data, namely from measurements of the energy gap. Indeed, the quantity $\beta = 2\Delta(0)/T_c$ depends on the value of λ_{ph}. For example, $\beta_{BCS}=3.52$ (weak coupling) $\beta_{Pb} \simeq 4.3 (\lambda \simeq 1.5)$, $\beta_{Hg} \simeq 4.5$ $(\lambda \simeq 1.6)$, $\beta_{Pb-Bi} \simeq 5 (\lambda \simeq 2)$.

The magnitude of the energy gap has been determined by infrared spectroscopy and various types of tunneling (see e.g. [3]). Although there is some variation in the data that have been reported, the majority corresponds to $\beta \lesssim 5$ (our analysis corresponds to the single-gap picture, or to the situation when $\ell < \xi_o$). This means that λ_{ph} for the La-Sr-Cu-O system does not exceed the value of $\lambda_{ph} \simeq 2$ (et. [16], see above). However, this is not sufficient to provide the experimentally observed $T_c \simeq 40K$. This temperature requires $\lambda_{ph}=5$ (see above).

Hence, we come to the conclusion that the electron-phonon interaction plays an important role in La-Sr-Cu-O, as manifested by various experimental data (see above), but, nevertheless, there is need for an additional mechanism of attraction between the carriers. We think that the electron-plasmon interaction is an additional mechanism which, jointly with the strong electron-phonon coupling, is responsible for high T_c superconductivity.

Plasmon branches corresponding to the poles of $\Gamma_{PL}(\omega, q)$ appear in the region $\omega > qv_F$. The region $\omega < q^vF$ does not contain any singularities of $\Gamma_{PL}(\omega, q)$. In this region, one can use static approximation and $I_{PL}(\omega, q)$ represents the usual screening. As a result, we obtain:

$$\Delta(P_z,\omega_n)Z + T\sum_{\omega_n'}\int d\Omega\left\{\left[\lambda_{PH}(\Omega,P_z,P_z')\frac{\Omega^2}{\Omega^2+(\omega_n-\omega_n')^2} - V_c\theta(|\omega_n|-\omega_o)\right.\right.$$
$$\left.\left. + \lambda_{PL}(\Omega,P_z,P_z')\frac{\Omega^2}{\Omega^2+(\omega_n-\omega_n')^2}\right\}\frac{\Delta(\omega_n',P_z')}{|\omega'_n|}\right|_{T=T_c}.$$

The concept of coexistence means that the electron-phonon interaction plays an important role. The Coulomb repulsion is overcome mainly by the electron-phonon interaction. As for the plasmon contribution one can see directly from Eq. (26) that the electron-plasmon interaction provides an additional mechanism of electron-electron attraction and in the presence of electron-phonon interaction it leads to an additional increase in T_c.

Equation (4) can be written in the form

$$\Delta(P_z, \omega_n)Z=T\sum_{\omega_n'}\int d\Omega\left\{\chi(\Omega, P_z, P_z')\frac{\Omega^2}{\Omega^2+(\omega_n-\omega_n')^2}-V_c\theta(\omega_n-\omega_0)\frac{\Delta(\omega_n;P_z')}{\omega_n/}\right\}_{T=T_c} \quad (5)$$

where $\lambda=\lambda_{PH}+\lambda_{PL}$. The Eq. (5) is a generalization of usual Eliashberg's equation. The plasmons will appear as a modification of the usual function λ_{PH}.

One can see directly from Eq. (4) that the anisotropy of the Fermi surface [13] and the interaction lead to the anisotropy of the energy gap.

The behavior of the anisotropic energy gap and T_c in the presence of the anisotropic Fermi surface and several coupling mechanisms is a complex problem and will be analyzed in detail elsewhere. For a rough estimate one may use the expression obtained in [ ], (assumed that $\lambda_{PH}\neq 0$):

$$T_c = T_c^{PH}\left(\frac{\widetilde{\Omega}_{PL}}{T_c^{PH}}\right)^a$$

$$a = \frac{\lambda_{PL}}{\lambda_{PL}+\lambda_{PH}} \quad (6)$$

where T_c^{PH} is the critical temperature in the absence of the plasmon mechanism. One can see that the large value of the plasmon energy Ω_{pl} makes the plasmon contribution noticeable, even for small λ_{PL}. For example, if $\lambda_{Ph}\approx 2$ (this value corresponds to $2\Delta(0)/kT_c\simeq 5$ (see above) and we use our model of a polar phonon-plasmon hybridized density of states (15) $\lambda_{PL}\approx 0.3$, $\Omega_{PO}\approx 60$ meV, we obtain $Tc^{Ph}\approx 22$K and $Tc\approx 38$K. In the absence of phonon-plasmon hybridization and using an experimental value of 1 eV for the bulk plasmon frequency which is a lower limit for the 3D to 2D crossover, we estimate a $\lambda_{PL}\approx 0.2$ for $Tc\approx 38$K. It is clear that an increase of Ω_{PL} results in a decrease of λ_{PL}.

Plasmon-induced pairing can, therefore, make a noticeable change in T_c relative to Tc^{PH} even for small values of λ_{PL} and it arises from the large value of the plasmon frequency.

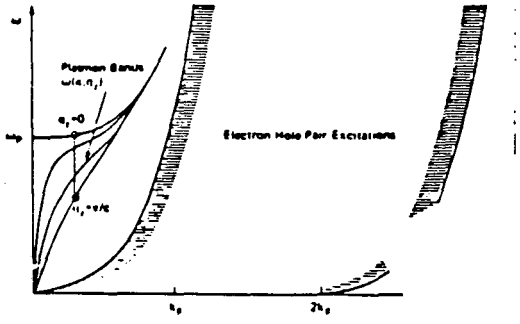
Although some factors such as exchange and vertex corrections [22] (in this work an isotropic 3D jellium model is considered, different from the case studied here) may result in some decrease of electron-plasmon coupling, we would like to stress that our concept of coexistence of strong electron-phonon coupling and the plasmon mechanism (see below) can explain the observed high transition temperature with weak electron-plasmon coupling.

In addition, the presence of different energy bands with different effective masses results in the appearance of additional plasmon bands breaches, the "demon" states.

Conclusion. In this paper we describe our approach to the theory of high T_c superconductivity. The dynamic part of the interaction between electrons in layered systems differs drastically from that in the usual 3D system. The collective excitations form a plasmon band, and the lowest branch corresponds to the maximum of the density of states.

Note that the plasmon edge measured by infrared technique corresponds to the upper plasmon branch (see Fig. 1), whereas the pairing is affected mainly by the lower branch. We studied also the hybridization of polar phonon and plasmon branches. The phonon-plasmon mechanism is described by the generalized Eliashberg equation. The large scale of the plasmon energy leads to a noticeable effect of plasmons upon T_c even for weak electron-

plasmon interaction.



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