Layer plasmons and high-T_c superconductivity

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We study a layered electron-gas model for the high-T_c copper oxides. The formation of plasmon bands by the interlayer Coulomb interaction is shown to lead to enhanced plasmon-induced electron pairing at the boundaries of the plasmon bands. We comment on the potential contribution of quasi-one-dimensional plasmons for the $YBa_2Cu_3O_{7-\delta}$ compounds. The concept of coexistence of phonon and plasmon mechanisms is discussed.

Among the several potential nonphonon mechanisms proposed to explain the dramatic increase in the superconducting transition temperatures in newly discovered, layered copper-oxide materials[1,2] is the plasmon mechanism.[3-7] The plasmons make an important contribution to the pairing, and high-T_c superconductivity in the new oxides is caused by coexistence of the phonon and nonphonon (plasmon) mechanism. Although no definitive exposition of the correct physical picture for these materials is available despite a large number of highly original and intriguing proposals,[3] we present in this paper some results that we believe add weight to the plasmon idea.

Specifically, we will show that it is not only the qualitatively different nature of electronic collective excitations (plasmons) in less than three dimensions that leads to their potentially important role in the layered copper-oxide materials, but also the formation of plasmon bands by the interlayer Coulomb interaction. This interaction redistributes the plasmon density of states to the boundaries of the plasmon branches, which enhances the coupling considerably. As is well known, the dispersion relation for the two-dimensional electron gas does not have a gap at $\kappa \to 0$.[8] In the region of small κ, Ω is proportional to $\kappa^{1/2}$. One can show that increasing κ leads to a linear dispersion relation $\Omega \sim \kappa$.[9] The interlayer Coulomb interaction leads to a noticeable modification of the simple two-dimensional (2D) dependence.[10-12] Layered crystals are characterized by a plasmon band $\Omega = f(\kappa, q_z)$, where κ, q_z are wave vectors in the planes and perpendicular to them, respectively. The z axis is chosen perpendicular to the layers (Fig. 1).

The values of Ω are restricted to lie between the upper and lower branches. These branches correspond to $q_z = 0$ and $q_z = \pi/c$ for the uppermost and lowest branches, respectively. In addition, we note that these boundary modes correspond to the in-phase motion of electrons on different planes ($q_z = 0$) and out-of-phase motion ($q_z = \pi/c$) on adjacent planes. Note that the layer spacing c is equal to half the lattice constant c_0 for $La_{2-x}Sr_xCuO_4$.

The plasmon spectrum of the layered electron gas has been studied recently because of the increasing interest in superlattices, in which conducting planes are separated by insulating planes.[10-12] We assume that we may use such a model for the layered copper oxides since their transport properties are highly anisotropic. Recent experimental evidence for 2D plasmons in single crystals of La_2NiO_4 was given in Ref. 13.

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

The upper branch corresponds to three-dimensional behavior, and the dependence of $\Omega(\kappa,0)$ is similar to the behavior of the usual three-dimensional sample. On the other hand, the behavior of the lowest branch $\Omega(\kappa,\pi/c)$ is entirely different. It is important to note that in the limit $\kappa_z \gg 1/c$, the interlayer interaction does not play an important role and we are dealing with a two-dimensional dispersion relation $\omega \sim \kappa$. There is a crossover from 3D→2D behavior in the region $\kappa_z \sim 1/c$. This crossover corresponds to a maximum in the density of states.[14] 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.

We now consider the interaction with the conduction

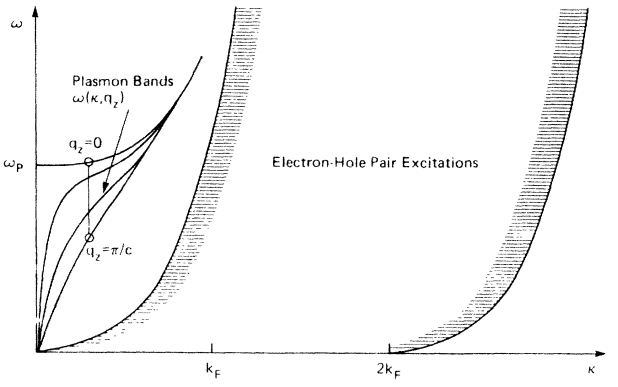

FIG. 1. Plot of the various plasmon branches and electron-hole pair excitations as a function of κ (absolute value of in-plane wave vector) and q_z for a layered electron gas.

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electrons with the entire set of collective excitations (plasmons) in the same manner we used earlier.[15]

Consider a simple model of a periodic array of two-dimensional conducting sheets and neglect electronic transition between layers. Such a model was studied in Refs. 10–12. $\Omega(\kappa,q_z)$ is described by the following relation (here n is the carrier aerial density; s is proportional to the Fermi velocity):

$$\Omega_{\pm}(\kappa,q_z)=\pm\left[s^2\kappa^2+\frac{2\pi ne^2}{m}\frac{\kappa\sinh(\kappa c)}{\cosh(\kappa c)-\cos(q_z c)}\right]^{1/2}. \tag{1}$$

It is easy to see that the derivative $\partial\Omega_+/\partial q_z$ at $q_z=0,\pm\pi/c$ vanishes. The singularity of $(\partial\Omega_+/\partial q_z)^{-1}$ implies a singularity of the plasmon density of states at both boundaries. This singularity is transformed into a sharp peak if we take into account a small interlayer hopping term.[12] The equation describing the pairing has the form (at $T=T_c$)

$$\Delta(\kappa,p_z;\omega_n)Z=T\sum_{\omega_{n'}}\int d^3p'\,\Gamma(q,p_z-p_z';\omega_n-\omega_{n'})\times\frac{\Delta(\kappa',p_z';\omega_{n'})}{\omega_{n'}^2+\xi'^2}\Bigg|_{T_c}. \tag{2}$$

$\omega_n=(2n+1)\pi T$, Δ is the order parameter, ξ' is the electron energy referred to the Fermi level, and Γ is the effective vertex describing the electron-electron interaction. Z is the renormalization function; $\mathbf{q}=\boldsymbol{\kappa}-\boldsymbol{\kappa}'$ is a two-dimensional momentum. Γ can be written as a sum

$$\Gamma=\Gamma_{\rm ph}+\Gamma_{\rm pl}. \tag{3}$$

Here $\Gamma_{\rm ph}=\lambda_{\rm ph}D_{\rm ph}(\omega_{\rm ph},\omega_n)$ is the phonon part and (from Ref. 16)

$$\Gamma_{\rm pl}=\lambda_{\rm pl}D_{\rm pl}(\Omega_{\rm pl},\omega_n)=\lambda_{\rm pl}\frac{\Omega_{\rm pl}^2}{\Omega_{\rm pl}^2+\omega_n^2}$$

describes the plasmon contribution to the pairing. This equation represents the usual Eliashberg equation if we study the effect of $\Gamma_{\rm ph}$ only.

The right-hand side of this equation can be written as a sum of two terms,

$$\Delta=\Delta_{\rm ph}+\Delta_{\rm pl}. \tag{4}$$

Let us focus on the plasmon term. The Fermi surface in our case has a cylindrical shape with $p_z^{\max}=\pi/c$. Using a cylindrical system of coordinates and integrating over ξ', we obtain

$$\Delta_{\rm pl}(\kappa,p_z;\omega_n)Z=\pi T\sum_{\omega_{n'}}\int dq\,dq_z\,\tilde{\lambda}(q,q_z)\frac{\Omega_{\rm pl}^2(q,q_z)}{\Omega_{\rm pl}^2(q,q_z)+(\omega_n-\omega_{n'})^2}\frac{\Delta(p_z+q_z,\omega_{n'})}{|\omega_{n'}|}\Bigg|_{T=T_c}. \tag{5}$$

We made a transformation $\phi\rightarrow q$ and introduced

$$\tilde{\lambda}(q,q_z)=\lambda_{\rm pl}(q,q_z)(4k_F^2-q^2)^{-1/2}.$$

The integration over q_z is limited to the range $p_z-2\pi/c<q_z<p_z$.

Let us introduce curves of constant plasmon frequency defined by the equation $\Omega(q,q_z)=\text{const}$. Making a transformation to the integration over these curves and Ω, we obtain after setting $\kappa=\kappa_F$,

$$\Delta_{\rm pl}(p_z,\omega_n)=\pi T\sum_{\omega_n'}\int d\Omega\,\tilde{G}_{\rm pl}(\Omega)\frac{\Omega^2}{\Omega^2+(\omega_n-\omega_n')^2}\times\frac{1}{|\omega_{n'}|}\Bigg|_{T=T_c}, \tag{6}$$

where

$$G_{\rm pl}(\Omega)=\int dl\,\tilde{\lambda}(q,q_z)v_1^{-1}\Delta(p_z+q_z,\omega_{n'})$$

and

$$v_1=[(\partial\Omega/\partial q)^2+(\partial\Omega/\partial q_z)^2]^{1/2}.$$

The integration is taken over the infinite set of curves $\Omega(q,q_z)=\omega_i$ $(i=1,2,\ldots,N)$ (see Fig. 2).

It is important that the quantity v_1^{-1} has a maximum at $q_z=\pi/c$, because the derivative $\partial\Omega/\partial q_z$ is equal to zero in this region (see above). This flat region of the plasmon branch makes a major contribution to the integral. Therefore, the main contribution to the pairing comes from the region $q_z=\pi/c$. This region corresponds to the lowest branch of the plasmon band, and this branch differs in a striking way from the three-dimensional branch.

The integral $\Delta_{\rm pl}(p_z,\omega_n)$ contains contributions of the entire frequency range up to $\Omega_{\rm pl}(q_c)$ where $\Omega_{\rm pl}(q)$ is determined by the lowest dispersion curve of the plasmon branches (see Fig. 1) and q_c is a cutoff momentum. If the function $\Omega_{\rm pl}(q)$ has a region of $q\sim q_0$ with a Van Hove-type singularity, where $\partial\Omega_{\rm pl}/\partial q=0$ (such a situation appears, for example, by hybridization of the plasmon and phonon modes; see Ref. 15), then this region of q and the corresponding frequency $\omega(q)$ play a major role.

Plasmon branches corresponding to the poles of $\Gamma_{\rm pl}(\omega,q)$ appear in the region $\omega>qv_F$ and $\Gamma_{\rm pl}(\omega,q)$ is an

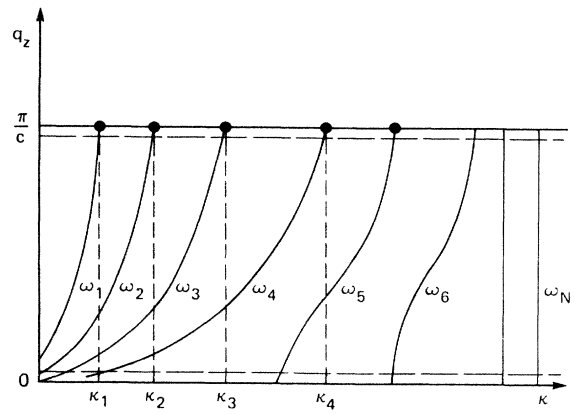

FIG. 2. Schematic plot of the constant frequency surfaces $\Omega(\kappa,q_z)$ with $\Omega_1<\cdots<\omega_N$.

analytic continuation of the function $\Gamma_{\rm pl}(\omega_n,q)$. The region $\omega < qv_F$ does not contain any singularities of $\Gamma_{\rm pl}(\omega,q)$. In this region one can use a static approximation and $\Gamma_{\rm pl}(\omega,q)$ represents the usual screening. This term (a more detailed analysis will be described elsewhere)[17] can be combined with the usual phonon term, and we obtain

$$\Delta(p_z,\omega_z)Z = T\sum_{\omega_n'}\int d\Omega \left[\left(\lambda_{\rm ph}(\Omega,p,p_z')\frac{\Omega^2}{\Omega^2+(\omega_n-\omega_{n'})^2} - V_c\Theta(|\Omega|-\omega_0) \right) + \lambda_{\rm pl}(\Omega,p,p_z')\frac{\Omega^2}{\Omega^2+(\omega_n-\omega_{n'})^2} \right] \frac{\Delta(\omega_{n'},p')}{|\omega_n'|} \quad . \tag{7}$$

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. (7) 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.

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 Ref. 18,

$$T_c = T_c^{\rm ph}\left(\frac{\tilde{\Omega}_{\rm pl}}{T_c^{\rm ph}}\right)^{\alpha}, \quad \alpha = \frac{\lambda_{\rm pl}}{\lambda_{\rm pl}+\lambda_{\rm ph}} \quad , \tag{8}$$

where $T_c^{\rm ph}$ is the critical temperature in the absence of the plasmon mechanism. One can see that the large value of the plasmon energy $\tilde{\Omega}_{\rm pl}$ makes the plasmon contribution noticeable, even for small $\lambda_{\rm pl}$. For example, if $\lambda_{\rm ph}\approx 2$ [this value corresponds to $2\Delta(0)/k_BT_c\approx 5$ (Ref. 18)] and we use our model of a polar phonon-plasmon hybridized density of states[15] $\lambda_{\rm pl}\approx 0.3$, $\Omega_{\rm pl}\approx 60$ meV, we obtain $T_c^{\rm ph}\approx 22$ K and $T_c\approx 38$ K. In the absence of phonon-plasmon hybridization and using an experimental value of 1 eV for the bulk plasmon frequency,[19] which is a lower limit for the 3D to 2D crossover, we estimate a $\lambda_{\rm pl}\approx 0.2$ for $T_c\approx 38$ K. It is clear that an increase of $\Omega_{\rm pl}$ results in a decrease of $\lambda_{\rm pl}$.

Plasmon-induced pairing can, therefore, make a noticeable change in T_c relative to $T_c^{\rm ph}$ even for small values of $\lambda_{\rm pl}$, and it arises from the large value of the plasmon frequency. Although we have used the random-phase approximation (RPA) in our analysis, it has been shown in Refs. 20 and 21 that one can go beyond the RPA with only changes in the plasmon dispersion relations. We will return to this point in a forthcoming paper.[17]

Although some factors such as exchange[22] and vertex corrections[23] (in this work an isotropic 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.

Our model of layer plasmons is especially appropriate for the $La_{2-x}(Sr,Ba)_xCuO_4$ compounds. In connection with the structure of $YBa_2Cu_3O_7$, we note that in addition to the two-dimensional Cu—O conducting sheets, there are also additional planes consisting of one-dimensional chains. The plasmon spectrum of such systems is very peculiar and there are two crossover regions, namely from one dimensional to two dimensional in the plane of chains, and from two dimensional to three dimensional between sets of planes. In addition, the presence of different energy bands with different effective masses results in the appearance of additional plasmon bands branches, the "demon" states.[24]

Similar to considerations made earlier about crossover from three-dimensional to two-dimensional behavior and resulting increase in the plasmon density of states, we suggest that both the 1D-to-2D and 2D-to-3D crossover regions will lead to enhanced plasmon densities of states (at the corresponding frequencies) and hence T_c. In addition, we would like to stress that the carriers forming the quasi-one-dimensional bands have heavier masses and small carrier concentration in the chains (which is different from the carrier concentration in the planes). As a result of both of these effects their effective three-dimensional plasma frequency $\omega_p^2 = 4\pi ne^2/m_{\rm chain}$ is expected to be small relative to the Fermi energy of the carriers in the planes. It results in strong coupling between the carriers in the planes and quasi-one-dimensional plasmons. This fact may be the origin of the increase in transition temperature of the 1-2-3 material compared to the $La_{2-x}Sr_xCuO_4$ materials. For this situation the pairing picture is similar to the usual electron-phonon problem as the plasma frequency ω_p^2 is small compared to E_F.

We have shown in this paper that treating the plasmons of the layered cuprites more realistically supports and extends the single two-dimensional plane model. The qualitative nature of the contribution to electron pairing by the lowest plasmon branch resembles the pure two-dimensional case, but adds strength in the low-frequency region because of the peak in the plasmon density of states. Additional contributions to pairing from quasi-one-dimensional plasmon branches and possibly the effects of crossover from 3D to 2D to 1D have been pointed out as the possible origin of higher T_c in the $YBa_2Cu_3O_7$ compounds.

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[1]T. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).
[2]M. K. Wu, J. R. Ashburn, C. J. Torng, P. H. Hou, R. L. Meng, L. Gao, Z. J. Huang, Y. Q. Wang, and C. W. Chu, Phys. Rev. Lett. **58**, 908 (1987).
[3]For a summary, see, for example, *Novel Superconductivity,* edited by S. A. Wolf and V. Z. Kresin, proceeding of the Berkeley Conference (Plenum, New York, 1987); or *High Temperature Superconductivity* (American Institute of Physics, New York, 1987).
[4]V. Z. Kresin, Proceedings of the Material Research Society Meeting, Anaheim, 1987 (unpublished), p. 19; Phys. Rev. B **35**, 8716 (1987).
[5]D. H. Lee and A. Ihm, Solid State Commun. **62**, 811 (1987).
[6]J. Ruvalds, Phys. Rev. B **35**, 8869 (1987).
[7]J. Ashkenazi, C. G. Kuper, and R. Tyk, Solid State Commun. **63**, 63 (1987).
[8]F. Stern, Phys. Rev. Lett. **18**, 546 (1967).
[9]T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).
[10]P. B. Visscher and L. M. Falicov, Phys. Rev. B **3**, 2541 (1971).
[11]A. L. Fetter, Ann. Phys. (N.Y.) **88**, 1 (1974).
[12]D. Grecu, Phys. Rev. B **8**, 1958 (1973); S. Das Sarma and J. J. Quinn, *ibid.* **25**, 7603 (1982); A. C. Tselis and J. J. Quinn, *ibid.* **29**, 3318 (1984); J. K. Jain and P. B. Allen, Phys. Rev. Lett. **54**, 2437 (1985); G. F. Giuliani and J. J. Quinn, *ibid.* **51**, 919 (1983); P. Hawrylak, J.-W. Wu, and J. J. Quinn, Phys. Rev. B **32**, 4272 (1985).
[13]J. M. Bassat, P. Odier, and F. Gervais, Phys. Rev. B **35**, 7126 (1987).
[14]L. D. Landau and E. M. Lifshitz, *Statistical Physics,* 2nd and revised ed. (Addison-Wesley, Reading, MA, 1976), p. 210.
[15]V. Z. Kresin and H. Morawitz, in *Novel Superconductivity,* edited by S. A. Wolf and V. Z. Kresin (Plenum, New York, 1987).
[16]A. W. Overhauser, Phys. Rev. B **3**, 1888 (1971); B. I. Lundquist, Phys. Kondens. Mater. **6**, 206 (1967).
[17]V. Z. Kresin and H. Morawitz, Superconductivity (to be published).
[18]B. Geilikman, Z. V. Kresin, and N. Masharov, J. Low Temp. Phys. **18**, 241 (1975).
[19]P. E. Sulewski, T. W. Noh, J. T. McWhirter, and A. J. Sievers, Phys. Rev. B **36**, 5735 (1987).
[20]P. Vashista and K. S. Singwi, Phys. Rev. B **6**, 875 (1972).
[21]A. K. Rajagopal, Phys. Rev. B **15**, 4264 (1977).
[22]O. Entin Wohlman and H. Gutfreund, J. Phys. C **17**, 1071 (1984); H. Gutfreund and I. Unna, J. Phys. Chem. Solids **34**, 1523 (1977).
[23]H. Rietschel and L. J. Sham, Phys. Rev. B **28**, 5100 (1983); M. Grabowski and L. J. Sham, *ibid.* **29**, 6132 (1984).
[24]D. Pines, Can. J. Phys. **34**, 1379 (1956).