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Acoustic plasmon exchange in multilayered systems: II. Application to high-T_c superconductors

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Abstract. A theory for high-T_c superconductivity has been developed using the Eliashberg model on the basis that the attractive interaction is provided by the plasmon-mediated effective interaction between the charge carriers. Calculation of T_c using these interactions, presented in our preceding paper, shows that T_c should rise, with a saturation effect, with the number of CuO layers per unit cell, which is in agreement with observations in the Tl- and Bi-based compounds. Furthermore, this theory shows that a short coherence length is an essential requirement for superconductivity at high temperature.

Since the discovery of the high-T_c superconductor by Bednorz and Müller [1], several authors [2–4] have discovered that the thalium-based compound $Tl_2Ba_2Ca_2Cu_3O_{10+x}$ can superconduct at temperatures as high as 125 K. Almost at the same time Maeda *et al* [5] and Chu *et al* [6] showed that some bismuth-based compounds such as $Bi_2CaSr_2Cu_2O_{8+x}$ become superconducting below 115 K. Compositional and structural analyses [7–9] of these superconductors have revealed that CuO layers in these compounds are probably responsible for the origin of their superconductivity. It has also been shown that the T_c in these materials depend on the number of CuO layers per cell, e.g. the thalium-based compound with only one CuO layer per cell has a T_c of 80 K; with two CuO layers its T_c is 105 K, whereas with three CuO layers it is raised to 125 K. Similar conclusions have also been drawn for the Bi-based compounds.

There has been much theoretical interest in discovering the mechanism that governs superconductivity in these materials. Although the various theoretical models so far differ in detail from each other, they seem to fall into two principal categories: one depending on the spin fluctuations of the charge carriers and the other on their charge fluctuations. For example, the work of Anderson [10] and Schrieffer *et al* [11] can be categorized as to belonging to the first group, while those of Varma *et al* [12], Kresin and coworkers [13], Askhenazi *et al* [14] and Ruvalds [15] belong to the second group. Both seem to have achieved limited success as far as explaining the available experimental data.

In this paper we adopt the second point of view and present a pairing theory based on the plasmon exchange model for the interaction between the charge carriers (holes or electrons, which will be called 'electrons' in this paper for uniformity) in the CuO layers of the high-T_c materials. Our first intention is to show that the Eliashberg model

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[16] applied to multilayered compounds, where the attractive interaction is chiefly mediated by plasmons, can yield a possible explanation of the high-T_c superconductivity of compounds such as Tl- and Bi-based cuprates. Then we intend to show that such an approach can also explain the rise in T_c with L, where L is the number of CuO layers per cell, with a saturation, indicating that T_c cannot be raised indefinitely with increasing L.

We model the cuprate superconductor as a system of CuO layers behaving like two-dimensional electron gases (2DEG) embedded in a medium of dielectric constant ε. In our previous paper [17] (hereafter referred to as I), we have calculated the effective interaction between the electrons within the framework of the RPA. These electrons interact with each other within the same layer as well as from layer to layer via an effective interaction involving plasmon exchanges among all layers. We believe that the interaction between the charge carriers located in two different layers will play a secondary role in the calculation of T_c compared to the intra-layer interaction, since the coherence length along the c-direction is smaller than that in the ab plane and it is also somewhat smaller than the inter-layer distance a [18]. For this reason we have only included the intra-layer interaction in this paper. However, it should be emphasized that our theory is not strictly two dimensional in the sense that the charge carriers within the same layer interact via plasmon exchanges in all layers. This interaction can be written as [17]

$$V(q,\omega)=\frac{2\pi e^2}{\varepsilon q}+\sum_{\kappa=1}^{L}\int_0^{\pi}\mathrm{d}\kappa'\,\frac{2\omega_\kappa(\kappa',q)|M_\kappa(\kappa',q)|^2}{\omega^2-[\omega_\kappa(\kappa',q)]^2} \tag{1}$$

or, as in I, in the more condensed 'standard' form as

$$V(q,\omega)=v_0+\mathbb{S}\frac{v_0 w_\kappa(\kappa')}{\beta-\beta_\kappa(\kappa')} \tag{2}$$

with $v_0=2\pi e^2/\varepsilon q$, $\beta=\omega^2/\sigma q$, $\beta_\kappa(\kappa')=\omega_\kappa^2(\kappa',q)/\sigma q$ and $\sigma=2\pi e^2 n_s/\varepsilon m^*$, and where q is a 2D-momentum vector parallel to the layers and the symbol $\mathbb{S}$ represents

$$\mathbb{S}\to\sum_{\kappa=1}^{L}\int_0^{\pi}\mathrm{d}\kappa'.$$

The poles in (1) or (2) yield the plasmon dispersion relations for the modes which are specified by κ and κ'. These modes are distributed into L bands labelled by κ. For $\kappa=1$ one has a pseudo-optical band, and for $\kappa=2,\ldots,L$, one has $L-1$ acoustic bands. All the bands present a low- and a high-energy limit corresponding to $\kappa'=\pi$ and to $\kappa'=0$, respectively. Note also that κ' can be considered as a third component of momentum q by writing $q_z=\kappa'/c$.

For the acoustic bands one has $\omega_\kappa(0,q)\approx\omega_\kappa(\pi,q)$. In other words, the acoustic bands are very narrow, and for small q one has $\omega\propto q$ (hence their name). Comparatively, the pseudo-optical band has a large width. At the low-energy side one has $\omega\propto q$ (acoustic limit for $\kappa'=\pi$) and at the high-energy side one has $\omega=$ constant (optical limit for $\kappa'=0$). This constant is $\omega_p=[(4\pi e^2/\varepsilon m^*)(n_sL/c)]^{1/2}$, i.e. the bulk plasmon frequency corresponding to a 3D electron density n_sL/c. As discussed in I, it is interesting to note that, if the interaction between layers of different cells is neglected (one cell limit), the width of all the bands strictly vanishes and, in particular, the pseudo-optical band tends to a single mode having a dispersion relation $\omega\propto q^{1/2}$ (the planar mode of an isolated 2DEG).

Before applying the effective interaction to the calculation of the T_c, let us first discuss the various parameters that have appeared in the above expressions. The only geometric parameters that appear in our theory are the distances between the layers: a small distance $a = 3.2$ Å between the L layers belonging to the same cell, and a larger distance of 11.55 Å between adjacent layers belonging to different cells. Hence the lattice constant is

$$c = La + b \tag{3}$$

with $b = 8.35$ Å. These numbers are yielded by the crystallographic data for the Tl-based compounds. Note that our c is one-half of the crystallographic c, when one takes account of the body centred character of the unit cell. Next, we take the area density $n_s = 0.004$ Å^{-2} which corresponds to a Fermi momentum $k_F = (2\pi n_s)^{1/2} = 0.16$ Å^{-1}, and to a bulk density of charge carriers of $n_s/a \approx 10^{21}$ cm^{-3}. This value of n_s is not confirmed in the literature, since no definite value has been reported until now. For other cuprates, some authors [19] suggest a k_F two times larger, which involves a much larger n_s. Other authors [20] consider models where n_s varies from layer to layer. Here we assume that n_s is the same in all layers. Finally, two other parameters have been used to describe our model completely: the effective mass m^* of the 'electrons' and the background dielectric constant ε. As in [20] we take $m^* = 4m$ and $\varepsilon = 12$, which seem to be the values accepted by most authors.

We now proceed to the calculation of the critical temperatures T_c for the Tl- (or Bi-)based cuprates using the Eliashberg model for strong-coupling superconductors. Because of the complexity of the original model, several approximate expressions have been developed by various authors [21–23, 13], which are valid in different ranges of strengths of the coupling. Most recently, Kresin [13] has shown that for practically all coupling strengths the critical temperature can reliably be obtained from

$$T_c = 0.25\,\tilde{\omega}[e^{2/\lambda_{eff}} - 1]^{-1/2} \tag{4}$$

where $\tilde{\omega}$ is the average boson (here plasmon) frequency

$$\tilde{\omega} = \langle \omega^2 \rangle^{1/2} \tag{5}$$

and λ_{eff} is the effective interaction strength [13]

$$\lambda_{eff} = (\lambda - \mu^*)/(1 + 2\mu^* + \lambda\mu^* t(\lambda)). \tag{6}$$

(In [13], Kresin describes function $t(\lambda)$ of (6) graphically for all λ, but analytically for $\lambda \leqslant 1$ and for $\lambda \geqslant 1$ only. For our region of interest, $0.5 < \lambda < 5$, we have adapted his analytical expression into $t(\lambda) = 0.75 + 0.8/(1 + \lambda) - 0.12(\lambda - 0.5)$ which agrees with his graphical data as well as his analytical expressions at the appropriate limits.)

The two quantities $\tilde{\omega}$ and λ are in turn calculated from two other quantities which are directly related to potential (1), namely

$$\lambda = N(0)\left\langle \sum_{\kappa,\kappa'} \frac{|M_\kappa(\kappa', q)|^2}{\omega_\kappa(\kappa', q)} \right\rangle_{FC} \tag{7}$$

and

$$\lambda\langle \omega^2 \rangle = N(0)\left\langle \sum_{\kappa,\kappa'} |M_\kappa(\kappa', q)|^2 \omega_\kappa(\kappa', q) \right\rangle_{FC} \tag{8}$$

where $\langle \ldots \rangle_{FC}$ denotes an average over the 2DEG Fermi curve and $N(0) = m^*/2\pi$ is the electron density of states on the Fermi curve. Here λ represents the average attractive

strength between the electrons, essentially mediated by the plasmons in our model, and $\tilde{\omega}$ is given by the square root of the ratio of (8) and (7).

We also need the average repulsive Coulomb strength

$$\mu = N(0)\langle v_s(q)\rangle_{FC} \tag{9}$$

where $v_s(q)$ represents the statically screened Coulomb interaction

$$v_s(q) = v_0(q)/(1 + v_0(q)\Pi(q, 0)) = 2\pi e^2/(\varepsilon q + 2m^* e^2) \tag{10}$$

$v_0(q)$ being the bare Coulomb interaction and $\Pi(q, 0)$ the static polarization propagator in a 2DEG. Since $\varepsilon q < 2\varepsilon k_F = 3.8$ Å^{-1} and $2m^*e^2 = 8/a_B = 15$ Å^{-1} (a_B is the Bohr radius), one can write $v_s(q) \approx \pi/m^*$, and one has $\mu \approx 1/2$. However, the repulsive strength entering (6) is not μ, but a renormalized μ^* given by

$$\mu^* = \mu/[1 + \mu \ln(E_F/\omega_0)] \tag{11}$$

where one introduces a retardation effect due to the various coupled boson fields appearing in the model. Energy ω_0 is generally presented as characterizing these bosons, but opinion about its choice is far from being unanimous, and hence also about the choice of μ^*. *A priori*, the contribution of the phonons should not be excluded from the model and ω_0 may be considered to be intimately related to these low frequency phonons. For instance, Ashkenazi *et al* [14], who, like us, consider an attraction mediated essentially by plasmon suggest $\mu^* = 0.3$. But phonons can be coupled to plasmons [13] and μ^* can drop to 0.1. Ruvalds [15] also has similar conclusions for μ^*. The only thing we may be sure of is that, if a system is a candidate for superconductivity, we must expect $\mu^* < \mu = 1/2$, and of course $\lambda > \mu^*$. Thus, for now, in our calculation, we keep μ^* as an undefined parameter with the proviso $0 < \mu^* < 1/2$.

The calculation of (7) and (8) leading to $\tilde{\omega}$ is facilitated by two relations given in Appendix A of I,

$$\sum_{\kappa=1}^{L} \frac{w_\kappa(\kappa')}{\beta_\kappa(\kappa')} = f(\kappa') \tag{12}$$

and

$$\sum_{\kappa=1}^{L} w_\kappa(\kappa') = \sum_{s=0}^{L-1} \alpha_s [c_s(\kappa')]^2 \tag{13}$$

with

$$c_s(\kappa') = e^{-saq} - 1 + f(\kappa')$$

and

$$f(\kappa') = \sinh cq/(\cosh cq - \cos \kappa').$$

The second member of (13) depends on L. According to Appendix A of I, one has

$$\alpha_0 = 1 \qquad \text{for } L = 1$$

$$\alpha_0 = \alpha_1 = 1 \qquad \text{for } L = 2$$

$$\alpha_0 = 1, \alpha_1 = 4/3, \alpha_2 = 2/3 \qquad \text{for } L = 3$$

$$\alpha_0 = \alpha_2 = 1, \alpha_1 = 3/2, \alpha_3 = 1/2 \qquad \text{for } L = 4.$$

with $\Sigma \alpha_s = L$. The κ'-integrations can then be performed exactly.

This gives

$$\sum_{\kappa,\kappa'} \frac{w_\kappa(\kappa')}{\beta_\kappa(\kappa')} = 1 \tag{14}$$

and

$$\sum_{\kappa,\kappa'} w_\kappa(\kappa') = \sum_{s=0}^{L-1} \alpha_s(e^{-2saq} - 1) + L \coth cq. \tag{15}$$

Hence

$$\lambda = \frac{2N(0)}{\pi} \int_{q_m}^{2k_F} dq \frac{v_0(q)}{[4k_F^2 - q^2]^{1/2}} \tag{16}$$

and similarly

$$\lambda\langle\omega^2\rangle = \frac{2N(0)}{\pi} \sigma \int_{q_m}^{2k_F} dq \frac{qv_0(q)S_L(q)}{[4k_F^2 - q^2]^{1/2}} \tag{17}$$

where $S_L(q)$ represents the right-hand member of (15)

First it is interesting to note that λ, as given by (16), does not depend on L. This is due to (14) which, in fact, is a sum rule related to the analytic properties of the RPA potentials. Moreover, the integral in (16) can be calculated exactly, giving

$$\lambda = (2N(0)e^2/\varepsilon k_F) \ln\{[2k_F + (4k_F^2 - q_m^2)^{1/2}]/q_m\}. \tag{18}$$

But a difficulty arises here. This integral diverges for $q_m \sim 0$ and this is the reason why a finite lower limit q_m has been explicitly introduced in (16). The situation is similar for $\lambda\langle\omega^2\rangle$ given by (17). The technique we propose to address this difficulty is to introduce a finite q_m (replacing 0) as the lower limit of integration in (16) and (17) to obtain finite results. As discussed below, the choice of a finite non-zero q_m can be justified physically, on the basis of the fact that the coherence lengths in these high-T_c superconductors are small.

To make our point let us calculate λ given by (16) and $\lambda\langle\omega^2\rangle$ given by (17) for various values of q_m extending from 0 to $2k_F$. Two points will facilitate our discussion. First, note that $\tilde{\omega}$ calculated from the ratio of (17) and (16) is finite and, as shown in figure 1, has a rather weak dependence on q_m, except for $q_m \sim 0$, where it tends rapidly to the limiting value given by

$$\langle\omega^2\rangle = (\sigma L/c) = (2\pi e^2/\varepsilon m^*)[n_s L/(La + b)] \tag{19}$$

(with an infinite slope at $q_m = 0$). For q_m large, i.e. approaching $2k_F$, $\tilde{\omega}$ tends slowly to the limit $[2k_F\sigma S_L(2k_F)]^{1/2}$. The second point to note is that λ_{eff} given by (6) is either independent of L or a slowly varying function of L since λ is independent of L, and μ^* can be only a slowly varying function of L via ω_0 which is related to the phonon fields. These two points allow us to consider $T_{cL} = C\tilde{\omega}_L$ (with C independent of L) as an expression depending, on the whole, only weakly on q_m, except for $q_m \sim 0$. But this region $q_m \sim 0$ is not physically acceptable for reasons which will be made clear from the following discussion.

Let us first calculate $C = T_{c2}/\tilde{\omega}_2$ as a function of q_m, using the experimental value $T_{c2} = 105$ K and $\tilde{\omega}_2$ as given in figure 1 for $L = 2$. This 'fitted' $C(q_m)$ (for $L = 2$), considered equally valid for all Ls, then yields $\lambda_{eff}(q_m) = 2/\ln[1 + (0.25/C)^2]$ by means of (4). Once $\lambda_{eff}(q_m)$ is known, μ^* can also be calculated as a function of q_m, using (6).

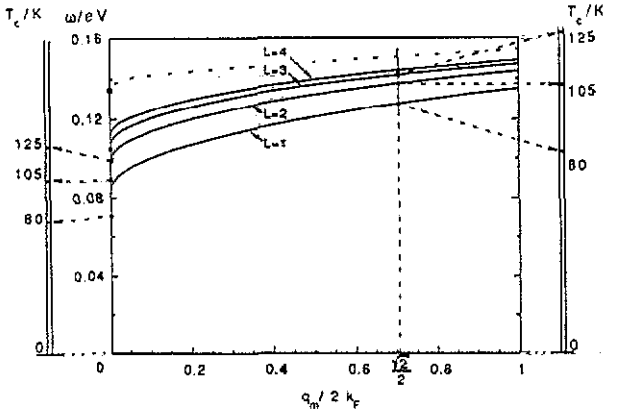

Figure 1. Plot of $\tilde{\omega}$ given by (5), (16) and (17) as a function of the lower limit of integration $q_m/2k_F$. For $q_m/2q_F = 0$ and $\sqrt{2}/2$, the relation $\tilde{\omega} \propto T_c$ is used to fit $\tilde{\omega}$ to T_c scales. The exact fit is realized for $T_c = 105$ K, the observed T_c for the Tl-based superconductor with $L = 2$. $\tilde{\omega}$ has a weak dependence in q_m except for $q_m \sim 0$ where it has a lower finite value with an infinite slope. The results presented in table 1 correspond to $q_m/2k_F = \sqrt{2}/2$.

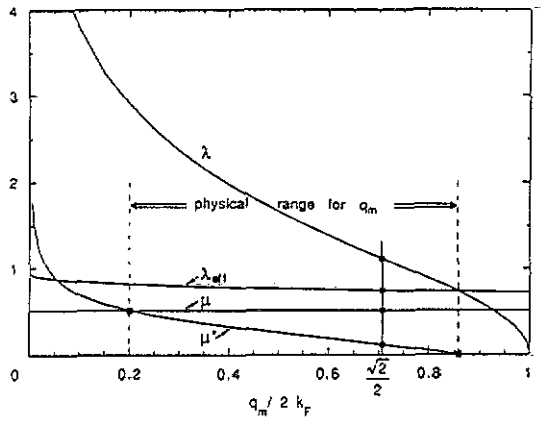

Figure 2. Plot of λ, λ_{eff}, μ and μ^* as functions of $q_m = 0$, λ diverges. The physically allowed range of q_m is shown by the double arrow. The values of λ, λ_{eff} and μ^* used in table 1 correspond to $q_m/2k_F = \sqrt{2}/2$.

In figure 2, we have plotted λ given by (18), the calculated λ_{eff} and μ^* as a function of q_m. It is interesting to note that $\mu^* < \lambda$ for all values of q_m, a prerequisite to get superconductivity. But since one must also have $0 < \mu^* < \mu = 1/2$, as indicated in figure 2, this requires $0.20 < q_m/2k_F < 0.86$ (or 0.06 Å$^{-1} < q_m < 0.27$ Å^{-1}). If q_m for a sample is outside this range, the set of equations (4)–(11) can no longer be applied, i.e. the sample will not be superconducting. This yields an argument for staying away from the region $q_m \sim 0$.

In order to see what value of q_m should be considered appropriate for a high-T_c superconductor, let us consider the following. If we calculate the integrand of (16) as a function of q, we find that it becomes infinite both at $q = 0$ and $q = 2k_F$ and has a minimum at $q = k_F\sqrt{2}$. It appears that a reasonable choice for q_m is around the value $k_F\sqrt{2}$ for the strong-coupling high-T_c superconductors. For this choice the integrand in (16) goes from its minimum value at the lower limit q_m where Cooper pairing, as expected, is weakest, up to an integrable infinity at the upper limit $q = 2k_F$, where the Cooper pairing is strongest. This choice also eliminates the region where the unphysical small q contributions are dominant. Furthermore, physically one would expect that the

Table 1. The calculated values for $\bar{\omega}$ as obtained from (16) and (17) and T_c as obtained from (4) are shown for $L = 1, 2, 3$ and 4. $q_m = k_F\sqrt{2} = 0.224\ \text{Å}^{-1}$, $\lambda = 1.11$, $\mu^* = 0.115$ and $\lambda_{eff} = 0.73$.

L	$\bar{\omega}$ (eV)	T_c (K)
1	0.128	97
2	0.138	105 (exact)
3	0.142	108
4	0.144	110

effective range of q_m should be of the order of inverse coherence length ξ_0, since charge carriers at distances larger than ξ_0 do not contribute significantly to Cooper pairing. It turns out that our choice for q_m is indeed of the order of the inverse coherence length ξ_0. To obtain an order of magnitude for ξ_0 we use the BCS relations $\xi_0 = k_F/\pi m^*\Delta$ for the coherence length and $\Delta = 1.76\, k_B T_c$ for the energy gap (with $T_c = 105$ K), and obtain $\xi_0 = 6$ Å or $1/\xi_0 = 1.04\, k_F$, which is of the order of our $q_m = k_F\sqrt{2}$. The measured coherence length for the high-T_c superconductors is generally reported as being of the order of 10 Å. This suggests that a somewhat lower value of q_m could also be chosen. As shown in figure 1, this would increase the relative range of the L-dependence of the T_c, bringing it closer to the observed range for the series of Tl-compounds. But too large a value of ξ_0 (as in the ordinary superconductors) will make $q_m \sim 0$, which will take us to the non-physical region for superconductivity (see figure 2). Let us emphasize the fact that the choice $q_m = k_F\sqrt{2}$, though very reasonable, is not unique. Any other choice of $q_m/2k_F$ between 0.20 and 0.86 (a range arising essentially from our model, as discussed before) would be acceptable and would not change the conclusions of this paper. The interesting point is that this range of values for q_m is precisely in agreement with the short coherence length found in the high-T_c superconductors.

In table 1, we quote the values of several quantities evaluated at our proposed $q_m = k_F\sqrt{2}$. These numbers correspond to the black dots of figures 1 and 2. Let us note that we obtain a reasonable value for $\mu^* = 0.12$, a value close to those estimated by several authors [13, 15]. Table 1 explicitly shows that T_c rises with the number of CuO layers per unit cell, even though our range of T_c values is smaller than the observed ones. This is probably due to our choice of the various parameters. Moreover, as shown by the dotted curve of figure 1, we have a saturation in T_c implying that T_c cannot be raised indefinitely by stacking more and more CuO layers in a cell [24–26]. Note that our theory is not contradictory to the model presented by DiStasio *et al* [20] where n_s is larger in the side layers of the cells than in the central layers. A depletion of n_s in the central layers in our theory may, in fact, improve some of our results, namely, by yielding a more extended range of T_c with increasing L.

Our most important conclusion is probably that the acoustic plasmon model, the one presented in our paper, may be a key to understanding the HTSCs. Our theory also explains the rise in T_c with the number of CuO layers per cell, with a saturation effect, as observed in the Tl- and Bi-based cuprate superconductors. Finally, our theory shows for the first time that high-T_c superconductivity is intimately connected with the short coherence length reported for these superconductors.

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