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LETTER TO THE EDITOR

An explanation for the rise in T_c in the Tl- and Bi-based high-temperature superconductors

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Abstract. Using the plasmon exchange model for the high-T_c superconductor, we show that the T_c rises with an increase in the number of CuO layers per unit cell, which is in agreement with recent observations in the Tl- and Bi-based compounds. Our calculation also shows that there is a saturation effect, i.e. that T_c cannot be raised indefinitely by increasing the number of CuO layers.

The recent discovery of superconductivity in the La–Ba–Cu–O system by Bednorz and Müller [1] in the region of 30 K has prompted a flurry of activity in the area of production of new materials with higher T_cs [2–7]. The first important breakthrough in reaching a T_c greater than the boiling point of liquid nitrogen was achieved by Wu *et al* [2] when they showed that $YBa_2Cu_3O_{7-x}$ with perovskite structure becomes superconducting at 90 K. The search for higher-temperature superconductors (HTSC) met with limited success until Hermann and co-workers and others [3–5] showed that the thallium-based compound $Tl_2Ba_2Ca_2Cu_3O_{10+x}$ can be made to superconduct at 125 K. Around the same time, Maeda *et al* [6] and Chu *et al* [7] discovered that the bismuth-based compound $Bi_2Ca_1Sr_2Cu_2O_{8+x}$ also achieves superconductivity at around 129 K. Subsequent compositional and structural analyses of these rare-earth-free superconductors [5, 8, 9] have determined several interesting features. First, it has been shown that in these compounds there are no CuO chains, and that CuO sheets are probably responsible for their superconductivity. These analyses have also shown that the T_c in these materials increase with the number of CuO layers per unit cell. For example, it has been shown that the thallium-bearing compound with a T_c of 90 K has one CuO layer, the material with a T_c of 95–108 K has two CuO layers, and the material with three CuO layers has the highest T_c of 125 K. It has been reported [10] that higher T_cs can be achieved by increasing the number of CuO layers, with perhaps a maximum T_c of 200 K. Our present letter addresses this issue.

Theoretically, several non-phononic models have been proposed to explain the high T_cs observed. Special mention should be made of Anderson's resonating valence bond (RVB) model [11], the Schrieffer *et al* spin bag model [12], the Varma *et al* charge excitation model [13] and the plasmon exchange models of Kresin [14], Ashkenazi *et al* [15] and Ruvalds [16]. In this letter we study the dependence of T_c observed in the Tl-

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and Bi-based compounds on the number of CuO layers, within the plasmon exchange model. We show that the T_c does indeed increase with the number of CuO layers. We also find that the increase of T_c with the number of layers achieves a saturation.

Here we will assume that the CuO layer forms a two-dimensional electron gas (2DEG) and that two electrons in a given layer can interact attractively by plasmon exchanges, either within that layer or via the various neighbouring layers. An isolated layer has only one plasmon mode with a dispersion relation $\omega \propto q^{1/2}$. Interacting layers have additional modes of acoustic nature ($\omega \propto q$) which enhance prospects for pairing. Our calculation is facilitated by the Eliashberg model [17] for strong-coupling superconductors. This model has been treated in an approximate way by various authors [18–20, 14] who provide prescriptions for calculating the T_c for such superconductors. Most recently Kresin [14] have shown that the critical temperature can be reliably obtained from

$$T_c = 0.25\tilde{\omega}(e^{2/\lambda_{eff}} - 1)^{-1/2} \tag{1}$$

where

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

$$\lambda_{eff} = (\lambda - \mu^*)/(1 + 2\mu^* + \lambda\mu^* t(\lambda)) \tag{3}$$

with the following definitions [19, 20, 14]

$$\lambda = N(0)\left\langle \sum_\kappa \frac{|M_k(q)|^2}{\omega_\kappa(q)} \right\rangle_{FC} \tag{4}$$

$$\langle\omega^2\rangle = \frac{N(0)}{\lambda}\left\langle \sum_\kappa |M_\kappa(q)|^2 \omega_\kappa(q) \right\rangle_{FC} \tag{5}$$

$$t(\lambda) \approx 0.75 + 0.8/(1 + \lambda) \qquad \text{for } \lambda \leqslant 1 \tag{6}$$

$$\mu^* = \mu/(1 + \mu \ln(\omega_{el}/\tilde{\omega})) \tag{7}$$

$$\mu = N(0)\langle v(q)\rangle_{FC} \tag{8}$$

where the square of the electron–plasmon matrix element $|M_\kappa(q)|^2$ and the plasmon frequency $\omega_\kappa(q)$, including the effect of plasmon exchange, can be obtained from the standard expression for the electron–electron interaction

$$V(q, \omega) = v(q) + \sum_\kappa \frac{2\omega_\kappa(q)|M_\kappa(q)|^2}{\omega^2 - \omega_\kappa^2(q)}. \tag{9}$$

In this equation, one has $v(q) = v_c(q)\Pi(q, 0) = 2\pi e^2/(q + 2m^* e^2) \approx \pi/m^*$, with $v_c(q)$ $(= 2\pi e^2/q)$ and $\Pi(q, 0)$ representing the bare Coulomb interaction and the static polarisation propagator in a 2DEG, respectively. In the above equations $\langle \ldots \rangle_{FC}$ denotes an average on the 2DEG Fermi curve and the summation signs run over the plasmon modes κ, that can be generated—the total number of which is related to the number of interacting layers in the sample.

By introducing this potential $v(q)$ in equation (8) and using $N(0) = m^*/2\pi$ for the density of states at the Fermi level, one obtains $\mu = 0.5$ for the Coulomb repulsion parameter. The attraction parameter λ can also be shown to be 0.5 when RPA potentials are used in (9) and (4) to describe the electron–plasmon–electron interaction. Parameter μ has then to be reduced to the effective repulsion parameter μ^* given by (7), otherwise T_c will be zero. Calculation of μ^*, however, requires the knowledge of a cut-off frequency

ω_{el}, the choice of which is far from being clear, at least for the HTSCs. Even for conventional superconductors, the calculation of this parameter μ^*, which has been widely discussed [18–20], has not been realised quite satisfactorily. In practice, μ^* has been evaluated by tunnelling measurements [20] for many of these superconductors and has been found to range from 0.092 to 0.117. Let us also note that the attractive role here is played by phonons and not by plasmons. For the HTSCs, where the phonon mechanism is apparently not the right one, μ^* has been treated up to now as an adjustable parameter [14–16] and has been quoted to range from 0.1 to 0.3. For our numerical computations, we have chosen $\mu^* = 0.1$, although a different choice of μ^* less than 0.5 will not alter the principal conclusions of this article.

With this choice of μ^* equations (1–3) and (6) yield

$$T_c = 0.0106\tilde{\omega} = 123(\mathrm{K/eV})\tilde{\omega} \tag{10}$$

and the calculation of T_c then boils down to the calculation of $\langle\omega^2\rangle$.

At this point it is interesting to mention that the value of $\langle\omega^2\rangle$ computed numerically below take simple analytical forms in two limiting cases. The first one corresponds to the situation where the conducting layers are separated by a large distance (or separated by intercalation layers with a large dielectric constant). In this case which corresponds to a system of non-interacting layers one has $\langle\omega^2\rangle = (8e^2/m^*)(2\pi n_s)^{3/2}$ where n_s is the electron density in the 2DEG. The other situation corresponds to a set of layers separated by a small distance a ($a \ll (8\pi n_s)^{-1/2}$) and thus strongly interacting via the plasmon exchange, and one has $\langle\omega^2\rangle = 2\pi e^2 n_s/m^* a$. These relations show why most of the layered compounds, namely the transition metal dichalcogenides, are not HTSCs, irrespective of whether their λ and μ^* take on values appropriate for occurrence of superconductivity. In general, the distance a is too large, the density n_s is too low (but may be increased by intercalation doping [21]) and the effective mass m^* is also too large due to narrow d-bands [22]—contributing to non-occurrence of superconductivity at high temperatures. Furthermore, low-energy 2DEG excitations like plasmons requiring highly laminar electronic properties do not seem to exist in most of these dichalcogenides as indicated by their band structure calculations [22], and when superconductivity occurs in these compounds it can be explained on the basis of phonons.

Let us now proceed to the calculation of T_c in the Tl- and Bi-based HTSCs.

(i) We first consider the case of a single CuO layer per unit cell, as is found in the $Tl_2Ba_2CuO_6$ compound. This situation then corresponds to an infinite number of CuO layers (2DEG) separated by the lattice constant c which for our calculation has been taken to be 24 Å [9]. For this case, the interaction between two electrons on the same layer, via plasmon exchange in all layers, can be shown to be [23]

$$V_{1\infty}(q, \omega) = \frac{v_c(q)S_1(q)}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}\kappa}{A_1(q, \omega) - \cos\kappa} \tag{11}$$

where

$$\begin{aligned} S_1(q) &= \sinh cq \\ A_1(q, \omega) &= \cosh cq - \sinh cq/\beta(q, \omega) \\ \beta(q, \omega) &= -(v_c(q)\Pi(q, \omega))^{-1} \approx m\omega^2/(2\pi e^2 n_s q). \end{aligned} \tag{12}$$

Comparing (11) with the standard expression (9), $|M_\kappa(q)|^2$ can be determined and introduced into (3), which is then evaluated to obtain $\tilde{\omega} = 0.764$ eV. At this point it

should be mentioned that all calculations in this paper have been carried out by assuming the electron (or hole) effective mass $m^* = m$, Fermi momentum $k_F = (2\pi n_s)^{1/2}$ with $n_s = 4 \times 10^{13}\,\mathrm{cm}^{-2}$. For our chosen parameters, we calculate $T_{c1\infty} = 94$ K which agrees with the one observed in the TlBaCuO sample.

(ii) Let us now calculate the critical temperature for the sample where there are two CuO layers per unit cell. This calculation obviously corresponds to the $Tl_2CaBa_2Cu_2O_{8+x}$ sample where the lattice constant c has been identified to be about 29 Å [4, 5]. For this case, the RPA electron–plasmon–electron interaction $V_{2\infty}(q, \omega)$ is given by an expression similar to (11) where S_1 and A_1 are replaced, respectively, by [23]

$$S_2(q, \omega) = \sinh cq - (2/\beta)\sinh aq \sinh(c-a)q$$

$$A_2(q, \omega) = \cosh cq - (2/\beta)\sinh cq + (2/\beta^2)\sinh aq \sinh(c-a)q \qquad (13)$$

with β given in (12). Here a is the separation between two CuO layers within the same cell, which for this calculation has been chosen to be 3.5 Å. A calculation similar to the one above yields $\tilde{\omega} = 0.822$ eV. Substitution of this ω in (10) gives us $T_{c2\infty} = 101.2$ K. Comparing this with $T_{c1\infty}$ we notice that the T_c obtained from the two-layer system is greater than the T_c for the one-layer system, which agrees with the experimental data [3–5].

Before proceeding to calculate T_c for the three-layer system, it is interesting to calculate the T_c of two isolated 2DEG layers separated by a distance a, to see how exclusion of inter-cell-layer interactions modifies the T_c. For this case there are only two plasmon modes with [23]

$$V_2(q, \omega) = \frac{v_c\beta}{2}\left(\frac{1+\gamma}{\beta-1-\gamma} + \frac{1-\gamma}{\beta-1+\gamma}\right) \qquad (14)$$

where β is given by (12) and where $\gamma = e^{-aq}$ [24]. The first mode corresponding to $\beta = 1 + \gamma$ is a proper 2DEG plasmon ($\omega \propto q^{1/2}$ for small q), and the second one corresponding to $\beta = 1 - \gamma$ is an acoustic plasmon ($\omega \propto q$). With the proper identification of $|M_1(q)|^2$ and $|M_2(q)|^2$, we have calculated $\tilde{\omega} = 0.818$ eV. This value when substituted in (10) gives us $T_{c2} = 100.7$ K. Note that this T_c, calculated for two isolated CuO layers, is almost the same as the one obtained above for a system with an infinite number of double layers separated by the lattice constant c [25]. Thus we conclude that for the purposes of calculation of T_c inter-cell-layer interactions can be neglected.

(iii) Here we calculate T_c for the three- and four-2DEG layers per unit cell system. The three-layer system corresponds to the case of $Tl_2Ba_2Ca_2Cu_3O_{10+x}$ which has been discovered to have three Cu-perovskite-like layers per unit cell with the lattice constant $c \approx 36$ Å [5], and the four-layer system has not been realised yet. Here also we can only consider isolated three- and four-layer systems, ignoring the inter-cell-layer couplings, because of the large values of c. Interestingly enough, the electron–electron interaction on the side layers happens to be different from that on the middle layer(s) as shown in the following equations [23]

$$V_{3s}(q, \omega) = \frac{v_c\beta}{2}\left(\frac{\beta(\beta-1)}{(\beta-1)^2 - \gamma^2(\beta-1) - 2\gamma^2} + \frac{\beta}{\beta-1+\gamma^2} - 2\right) \qquad (15a)$$

$$V_{3m}(q, \omega) = \frac{v_c\beta(\beta-1+\gamma^2)}{(\beta-1)^2 - \gamma^2(\beta-1) - 2\gamma^2} \qquad (15b)$$

$$V_{4s}(q,\omega)=\frac{v_c\beta}{2}\left(\frac{\beta(\beta-1-\gamma)}{(\beta-1)^2-\gamma(1+\gamma^2)(\beta-1)-\gamma^2(1+2\gamma)}+\text{idem}(\gamma\to-\gamma)-2\right) \tag{16a}$$

$$V_{4m}(q,\omega)=\frac{v_c\beta}{2}\left(\frac{(1+\gamma)(\beta-1+\gamma^2)}{(\beta-1)^2-\gamma(1+\gamma^2)(\beta-1)-\gamma^2(1+2\gamma)}+\text{idem}(\gamma\to-\gamma)\right). \tag{16b}$$

These systems have one 2DEG plasmon mode plus 2 (or 3) acoustic modes.

Following the procedure described in (i) and (ii), the critical temperatures for the side and middle layers of these systems are calculated to be $T_{c3s}=103$ K, $T_{c3m}=108$ K, $T_{c4s}=104$ K and $T_{c4m}=111$ K. The presence of two critical temperatures for each case suggests that the whole sample may not become superconducting at a single temperature, but rather in two stages. This conclusion is similar to that of Ihm and Yu [26] who show that a high-T_c system can have more than one gap depending on the number of CuO layers per unit cell. However, even the smallest Josephson coupling between different layers, which we have not included in our calculation but is physically or chemically impossible to avoid, will lead to a single combined three-dimensional critical temperature. Notice that $T_{c4m}>T_{c3m}>T_{c2\infty}\approx T_{c2}>T_{c1\infty}$. This follows the experimental trends observed in the Tl- and Bi-based superconductors, even though the calculated values for the two- and three-layer systems are somewhat different, and the four-layer system has not been achieved experimentally. Our results indicate that even higher T_cs may be achieved by stacking more CuO layer per unit cell. However, it should be noted that $(T_{c4m}-T_{c3m})<(T_{c3m}-T_{c2})<(T_{c2}-T_{c1\infty})$ indicating a saturation effect, i.e. T_c cannot be increased indefinitely by stacking more and more CuO layers per unit cell. In fact, our calculation of T_c for the extreme case of an infinite number of CuO layers per unit cell gives a maximum $T_{c\infty}=118$ K, supporting the above conclusion.

In conclusion, we would like to emphasise the principal findings of this paper. First, our calculation, based on the plasmon exchange model, shows that the T_c for a sample should increase as the number of layers per unit cell is increased, thus verifying the recent experimental findings in the Tl- and Bi-based superconductors. Considering the crudeness of the choice of our parameters, any agreement of our results with available experimental data for one-, two- and three-layer systems is at most a happy coincidence. More importantly, however, our calculation shows a saturation effect in the value of T_c, i.e. T_c will attain a maximum value beyond which it cannot be increased by further stacking—a point which has been alluded to by several authors [10, 26]. Finally, it should be pointed out that although the plasmon exchange model has been used in our theory, it should be applicable to other phonon exchange type models proposed by various authors.

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[24] The calculation of V_2 can be performed directly or, as a check, by taking the limit of $V_{2\infty}$ for $c \to \infty$. A quick check of equations (14), (15) and (16) can be made by letting $\gamma \to 0$ and $\gamma \to 1$. For $\gamma = 0$, the distance between the successive layers becomes infinity and one obtains $V_n(q, \omega) = v_c(q)\beta/(\beta - 1) = v_c(q)/(1 + v_c(q)\Pi(q, \omega))$, which is the RPA result for an isolated layer. For $\gamma = 1$, the n layers in the unit cell collapse into a single layer and we have $V_n(q, \omega) = v_c(q)\beta/(\beta - n) = v_c(q)/(1 + nv_c(q)\Pi(q, \omega))$, which is again the RPA result for a single layer, where the electron density is multiplied by n.

[25] Similarly $T_{c1\infty} = 94$ K should be compared with a calculation of T_{c1} related to a system of one independent CuO layer where the intra-layer potential has the form $V_1(q, \omega) = v_c\beta/(\beta - 1) = v_c/(1 + v_c\Pi)$ and which yields a critical temperature $T_{c1} = 92$ K. Note that our choice of $\mu^* = 0.1$ has been dictated by the fact that it yields a T_{c1} which is close to the experimental value.

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