Electronic plus phonon-exchange mechanism for high-temperature superconductivity in layered crystals

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Abstract. A general mathematical formulation is developed for calculating the effective electron–electron interaction in layered crystals like $YBa_2Cu_3O_{7-\delta}$, and for finding the resulting superconducting transition temperature T_c in such systems within the framework of the conventional BCS pairing arising from various possible excitations in the medium. This differs considerably from the usual case of an effective three-dimensional homogeneous system, and should be relevant in the calculation of T_c for the new class of high-T_c perovskites in which oxygen deficiencies in Cu-O layers and their distribution in the crystal play a crucial role. The explicit form of the effective interaction $V_{jj}(q_t, \omega)$ in a given layer j in the unit cell of the crystal is found to be determined not only by the true polarization function $\pi_j(q_t, \omega)$ of that layer, but also of other layers. The exchange of electronic excitations of a nearby insulating layer by carriers in a conducting layer thus becomes possible to get high T_c, with or without the usual phonon exchange.

Keywords. High temperature superconductivity; layered materials; electronic plus phonon mechanism for superconductivity; BCS pairing for high T_c superconductors.

1. Introduction

The discovery of superconductivity with the transition temperature T_c greater than 30 K in La-Ba-Cu-O system by Bednorz and Muller (1986) by the end of 1986, and the remarkable achievement (Wu *et al* 1987; Zhao *et al* 1987; Ganguly *et al* 1987a, b; Sampathkumaran *et al* 1987; Dhar *et al* 1987; Umarji *et al* 1987) of above 90 K superconductivity in $YBa_2Cu_3O_{7-\delta}$ and other similar oxygen deficient perovskites by March 1987, have given rise to phenomenal interest in the old field of high temperature superconductivity (see, for an earlier review, Ginzburg and Kirzhnits 1982). Various theoretical models (Rice 1987) involving both the conventional BCS type of pairing (Mattheiss 1987; Weber 1987; Jagadish and Sinha 1987; Varma *et al* 1987; Ruvalds 1987; Lee and Ihm 1987; Kresin 1987) and other types of phase transition (Anderson *et al* 1987; Emery 1987; Mohan and Kumar 1987) have recently been proposed as possible candidates for explaining such a high T_c. There is, of course, a general belief that for the BCS pairing of electrons at the Fermi surface arising from the attractive interaction in a very narrow energy range due to purely lattice phonon exchange, one cannot get T_c greater than about 40 K. Although, the theoretical validity of this result in the very strong coupling regime in which the dimensionless phonon-coupling constant λ_{ph} is much greater than 2, is still in doubt (Ginzburg and Kirzhnits 1982), at least in any

weak or moderate coupling theory, one has to go beyond the phonon exchange mechanism of superconductivity to obtain higher T_c, except possibly in the case of metallic hydrogen which has very high Debye phonon frequency. Starting from the early suggestions of Little (1964) and Ginzburg (1964) regarding high T_c-superconductivity due to the exchange of electronic excitations, instead of the usual phonon-exchange, in long organic molecules and metal-dielectric interfaces, respectively, the problem of high temperature superconductivity has been studied extensively for a long time within the framework of the conventional phase transition of the BCS theory. The order of magnitude calculation of T_c in a semiconductor-metal sandwich presented by Allender *et al* (1973a,b) was shown to be an overestimate (Rangarajan 1974; Rangarajan and Jha 1976; Srinivasan and Jha 1978), with the conclusion that such a structure can give high T_c only if the metal thickness is less than 2–3 Å. However, several other possibilities (Ginzburg and Kirzhnits 1982) for obtaining high T_c, including, e.g. our prediction of T_c in the range of 100 K in a two-band electron-hole system with carrier densities of about 10^{21} cm^{-3} and effective mass ratios of the two carriers greater than 8 (Bhattacharyya and Jha 1978; Srinivasan *et al* 1979) arising mainly from the acoustic-plasmon (i.e. electron-hole sound) exchange, have already been worked out within the conventional framework. It is, therefore, natural to ask ourselves whether the superconducting transition in the newly discovered 90 K superconductors is described by a completely different type of phase transition, e.g. by the resonating valence bond model of Anderson *et al* (1987), or it can still be explained within the conventional BCS framework with electronic exchange or/and phonon exchange mechanisms for the attractive interaction.

Because of the initial conflicting experimental data on various important physical parameters relevant to the transition, mainly due to uncontrolled but important variations in the preparation of the new ceramic superconducting materials with varying oxygen deficiencies, it has been difficult to examine critically most of the theoretical proposals presented recently. However, with improved reliability in experimental data, i.e. in the observation of the isotope effect in La-Ba-Cu-O system, consistent determination of the ratio $2\Delta/k_B T_c$, where Δ is the superconducting gap parameter, etc., one should soon reach a stage at which some of these possibilities can be set aside. As one examines the available experimental data today, one does not see any overwhelming reason to abandon our search for finding the correct mechanism for superconductivity in these new class of materials within the conventional BCS pairing theory. While one must continue to examine and explore possible alternative theories, there is still a great need for investigating more critically various possibilities in model systems, as close to the actual class of the 90 K superconducting materials as possible, within the conventional framework. It is in this spirit that we begin with this paper a theoretical investigation of superconducting transition due to the exchange of various excitations, both electronic and ionic, in crystals whose unit cell consists of approximately two-dimensional layers in the x-y plane (the plane of a and b axes) with relatively weak coupling between the planes in the vertical z-direction (c-axis). It is known that the periodic unit cell of $YBa_2Cu_3O_{7-\delta}$, $0 \leqslant \delta < 0.5$, can be conveniently described by six such layers, the crystal consisting of planes of Y, Cu-O, Ba-O, oxygen deficient Cu-O, Ba-O, Cu-O, Y, ... The layered structure and the amount of oxygen deficiency in Cu-O planes seem to control the value of T_c in a crucial sense. For such

a special 3-dimensional (quasi 2-dimensional) system, it is necessary to obtain the effective interaction between the electrons and the resulting superconducting T_c in a manner different from the usual approximately homogeneous systems. For a crystal with equally-spaced alternate metallic and insulating molecular layers, this point has already been discussed earlier by Bulaevskii and Kukharenko (1971).

In §2 of this paper, a mathematical formulation of the theory of superconducting transition in layered crystals is presented. Discrete Fourier representation has been used to solve the coupled equations for the effective electron-electron interaction between different layers in the crystal, which one obtains in a simple diagrammatic perturbation theory. Once the two-dimensional true polarization functions $\pi_j(q_t, \omega)$ for different charge carriers in each layer j are known, the effective interaction $V_{jj}(q_t, \omega)$ for electrons within the layer j can be obtained without any difficulty. The effective interaction $V_{jj}(q_t, \omega)$ is shown to contain contributions not only from the polarization function π_j of the layer, but also from the polarization function of the other layers in the unit cell. Thus a considerable enhancement of T_c or even the primary occurrence of the transition in a conducting layer becomes possible with the help of, e.g. exciton exchange in a nearby insulating layer. The nature of the polarizability functions π_j, including possible consequences are discussed in §3.

2. Mathematical formulation: Effective interaction in layered crystals and equation for T_c.

The first important step in the calculation of the superconducting transition temperature in any metal or alloy is the determination of the effective electron–electron interaction in the system. Although, in a crystal this involves the complete knowledge of the inverse dielectric tensor matrix $\varepsilon_{ij}^{-1}(\mathbf{q}+\mathbf{G}, \mathbf{q}+\mathbf{G}', \omega)$ in the reciprocal lattice vector **G**-space, it is often approximated by an effective 3-dimensional longitudinal dielectric function $\varepsilon^{-1}(q, \omega)$ of a homogeneous medium. In a layered or an anisotropic structure, this approximation can at best be made only for the motion in the plane of the layers (the *x-y* plane). In such a case, the relevant longitudinal dielectric function and the effective interaction are obtained in the form $\varepsilon^{-1}(q_t, \omega, z, z')$ and $V(q_t, \omega, z, z')$, respectively, where q_t is the magnitude of the 2-dimensional wave vector in the plane of the layers. Note that this effective interaction V, which we would like to calculate here, is between the carriers in the actual system, which could be either electrons or holes (or both), although we may continue to use the word "electrons". In what follows, we will formulate this problem by assuming that the layers in the crystal are vanishingly thin. If the actual spread of the charge distribution for these layers in the vertical direction becomes crucial, we would have to modify this approach suitably. Instead of discrete Fourier series used here, we will then have to use the usual continuous Fourier transform for solving the problem.

For definiteness, as an example, we will consider without any loss of generality the case of $YBa_2Cu_3O_{7-\delta}$, while formulating the method of obtaining effective interaction in a layered crystal (see figure 1). Let us label different layers perpendicular to the vertical *c*-axis by running integers *n*. In a given unit cell *N*, different layers may be
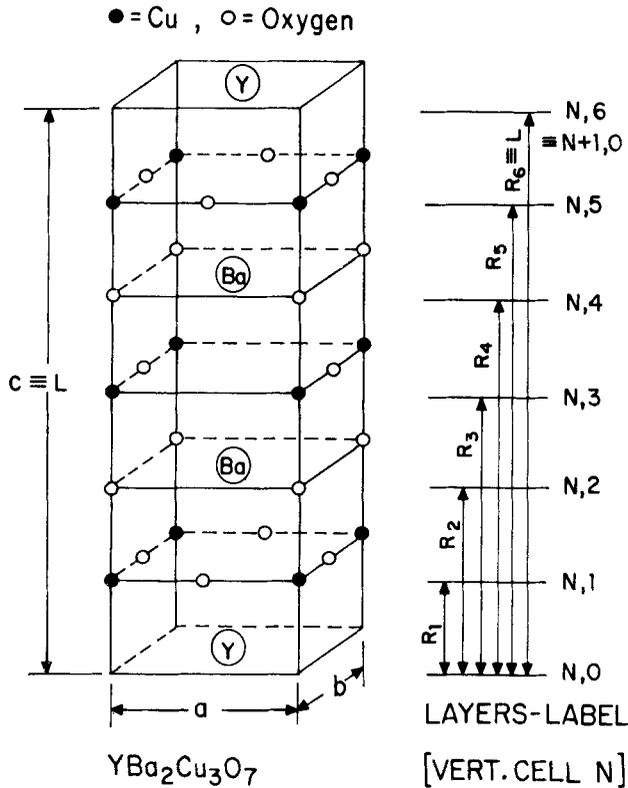
Figure 1. The unit cell of $YBa_2Cu_3O_7$ and labelling of different horizontal layers. The vertical distances between different layers in the crystal are also labelled. Here, approximately, $L = 11 \cdot 65$ Å.

labelled by N, j ($j = 0, 1, 2, 3, 4, 5, 6$), with the layer N, 6 same as $N + 1, 0$, because of the periodicity. This implies that the running label n can be rewritten as

$$n = 6N + j; \quad j = (0, 1, 2, 3, 4, 5); \quad N = 0, 1, 2, \ldots \tag{1}$$

where the z-coordinate of the nth layer is given by

$$z_n(N, j) = NL + R_j, \quad R_o \equiv 0 \tag{2}$$

where $L = R_6$ is the periodicity of the crystal in the vertical direction and R_j is the distance of the jth plane from the 0th plane in the unit cell. Although, the exact beginning for the numbering of layers and starting of unit cells are arbitrary, in any unit cell we assign $j = 0$ for the bottom Y-plane, $j = 1$ for the first full Cu-O plane, $j = 2$ for the first Ba-O plane, $j = 3$ for the oxygen deficient Cu-O plane, $j = 4$ for the second Ba-O plane, $j = 5$ for the second full Cu-O plane and $j = 6$ for the top Y-plane (see figure 1).

For fixed q_t and ω, the bare Coulomb interaction between electrons in $z - z'$ representation is given by

$$V^{(o)}(q_t, \omega, z_n - z_{n'}) \equiv V^{(o)}(q_t, n, n') = \frac{2\pi e^2}{q_t} \exp(-q_t|z_n - z_{n'}|) \tag{3}$$
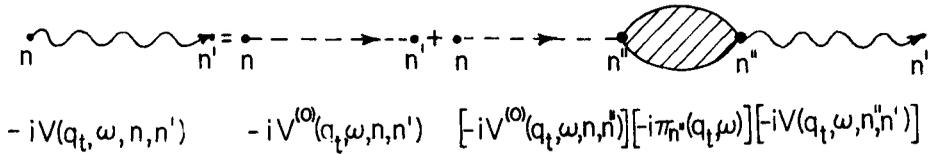
$$-iV(q_t, \omega, n, n') \qquad -iV^{(0)}(q_t, \omega, n, n') \qquad [-iV^{(0)}(q_t, \omega, n, n'')][-i\pi_{n''}(q_t, \omega)][-iV(q_t, \omega, n'', n')]$$

Figure 2. Perturbation diagrams to obtain the effective interaction V between the electrons (carriers) in different horizontal layers n and n'. $V^{(0)}$ corresponds to the bare Coulomb interaction (see text) and the running index $n = 6N + j$, $N = 0, 1, 2 \ldots \infty$, $j = 0, 1, 2, 3, 4, 5$ for six distinct layers in a given vertical cell N.

Note that in the usual 3-dimensional homogeneous case, a further Fourier transform of the above expression with respect to $z - z'$ leads to the well known form for the bare Coulomb interaction $4\pi e^2/q^2$, $q^2 = q_t^2 + q_z^2$. In a simple diagrammatic perturbation theory (see figure 2), the effective interaction V between the electrons is obtained by solving the equations

$$V(q_t, \omega, n, n') = V^{(0)}(q_t, n, n')$$

$$-\sum_{n''} V^{(0)}(q_t, n, n'')\pi_{n''}(q_t, \omega)V(q_t, \omega, n'', n'), \qquad (4)$$

where $\pi_n(q_t, \omega)$ is the polarization function (operator) of the nth layer, with the periodicity $\pi_{n+6} = \pi_n$, etc. In the random-phase approximation, this can be simply taken to be a sum of different contributions from *independent* carriers in the plane. If we redefine our interaction functions in terms of layer labels N, j, instead of n, as

$$V^{(0)}(q_t, 6N + j, 6N' + j') \equiv V_{jj'}^{(0)}(q_t, N, N')$$

$$= \frac{2\pi e^2}{q_t} \exp[-q_t|(N - N')L + R_{jj'}|], \qquad (5)$$

$$V(q_t, \omega, 6N + j, 6N' + j') \equiv V_{jj'}(q_t, \omega, N, N'); \quad R_{jj'} \equiv R_j - R_{j'}, \qquad (6)$$

(4) can be rewritten in the form

$$V_{jj'}(q_t, \omega, N, N') = V_{jj'}^{(0)}(q_t, N, N') - \sum_{N''=0}^{\infty} \sum_{j''=0}^{5} V_{jj''}^{(0)}(q_t, N, N'')\pi_{j''}(q_t, \omega)$$

$$\times V_{j''j'}(q_t, \omega, N'', N'). \qquad (7)$$

Using the discrete Fourier representation with respect to the variables $N - N'$, defined by

$$g(\theta) = \sum_{N-N'=-\infty}^{\infty} g(N - N') \exp[-i(N - N')\theta], \qquad (8)$$

$$g(N - N') = \int_0^{2\pi} \frac{d\theta}{2\pi} g(\theta) \exp[i(N - N')\theta]. \qquad (9)$$

Equation (7) can be reduced to the form

$$V_{jj'}(\theta) = V_{jj'}^{(0)}(\theta) - \sum_{j''=0}^{5} V_{jj''}^{(0)}(\theta) \pi_{j''} V_{j''j'}(\theta), \qquad (10)$$

where for brevity we have suppressed explicit q_t, ω dependences of V, $V^{(o)}$ and π. Here, θ/L corresponds exactly to the wavevector q_z of the usual Fourier transform representation, restricted to the first Brillouin zone. In terms of 6×6 matrices $V^{(o)}$, V and π, with matrix elements $V_{jj'}^{(o)}$ $V_{jj'}$ and $\pi_j \delta_{jj'}$, respectively, the above equation can be solved immediately in the form

$$V(q_t, \omega, \theta) = [I + V^{(o)}(q_t, \theta)\pi(q_t, \omega)]^{-1} V^{(o)}(q_t, \theta) \qquad (11)$$

where I is the 6×6 unit matrix. Explicitly, the matrix elements of $V^{(o)}$ are

$$V_{jj'}^{(o)}(q_t, \theta) = \begin{cases} \dfrac{2\pi e^2}{q_t} [\exp(-q_t R_{jj'})P(\theta) + \exp(q_t R_{jj'})N(\theta)]; & j > j' \\[2ex] \dfrac{2\pi e^2}{q_t} [\exp(q_t R_{jj'})P(-\theta) + \exp(-q_t R_{jj'})N(-\theta)]; & j < j' \end{cases} \qquad (12)$$

with

$$V_{jj'}^{(o)}(q_t, \theta) = V_{j'j}^{(o)}(q_t, -\theta) = V_{j'j}^{(o)*}(q_t, \theta), \qquad (13)$$

$$P(\theta) = \sum_{M=0}^{\infty} \exp(-q_t LM) \exp(-iM\theta)$$
$$= \exp(i\theta)[\exp(i\theta) - \exp(-q_t L)]^{-1}, \qquad (14)$$

$$N(\theta) = \sum_{M=1}^{\infty} \exp(-q_t LM)\exp(iM\theta)$$
$$= \exp(-q_t L)[\exp(-i\theta) - \exp(-q_t L)]^{-1}. \qquad (15)$$

Once the polarization functions $\pi_j(q_t, \omega)$ for the six layers are known, in principle (11)–(15) determine the effective interaction completely. For the required effective interaction for electrons or holes inside a given layer, we find

$$V_{jj}(q_t, \omega) \equiv V_{jj}(q_t, \omega, N, N) = \int_0^{2\pi} \frac{d\theta}{2\pi} V_{jj}(q_t, \omega, \theta)$$

$$= \sum_{j'=0}^{5} \int \frac{d\theta}{2\pi} [\varepsilon^{-1}(q_t, \omega, \theta)]_{jj''} V_{j''j}^{(o)}(q_t, \theta), \qquad (16)$$

where we have defined a 6×6 dielectric function matrix by the relation

$$\varepsilon(q_t, \omega, \theta) = I + V^{(o)}(q_t, \theta)\pi(q_t, \omega), \qquad (17)$$

the inverse of which is required to find the matrix $V(q_t, \omega, \theta)$, via (11). Explicitly, in terms of determinants of matrices $M^{\langle i,j \rangle}$ and ε, where $M^{\langle i,j \rangle}$ is obtained by replacing the ith column of ε by the jth column of $V^{(o)}$, i.e.

$$M_{j'j''}^{\langle i,j \rangle} \equiv \begin{cases} \varepsilon_{j'j''}, & j'' \neq i \\ V_{j'j}^{(o)}, & j'' = i \end{cases} \qquad (18)$$

the complete solution of (15) for V is given by

$$V_{ij}(q_t, \omega, \theta) = \det M^{\langle i,j \rangle}/\det \varepsilon. \tag{19}$$

For example, the complete form of $V_{33}(q_t, \omega, \theta)$ is
$V_{33}(q_t, \omega, \theta)$

$$= \det \begin{vmatrix} 1+v_o\pi_o & V_{01}^{(o)}\pi_1 & V_{02}^{(o)}\pi_2 & V_{03}^{(o)} & V_{04}^{(o)}\pi_4 & V_{05}^{(o)}\pi_5 \\ V_{10}^{(o)}\pi_o & 1+v_o\pi_1 & V_{12}^{(o)}\pi_2 & V_{13}^{(o)} & V_{14}^{(o)}\pi_4 & V_{15}^{(o)}\pi_5 \\ V_{20}^{(o)}\pi_o & V_{21}^{(o)}\pi_1 & 1+v_o\pi_2 & V_{23}^{(o)} & V_{24}^{(o)}\pi_4 & V_{25}^{(o)}\pi_5 \\ V_{30}^{(o)}\pi_o & V_{31}^{(o)}\pi_1 & V_{32}^{(o)}\pi_2 & v_o & V_{34}^{(o)}\pi_4 & V_{35}^{(o)}\pi_5 \\ V_{40}^{(o)}\pi_o & V_{41}^{(o)}\pi_1 & V_{42}^{(o)}\pi_2 & V_{43}^{(o)} & 1+v_o\pi_4 & V_{45}^{(o)}\pi_5 \\ V_{50}^{(o)}\pi_o & V_{51}^{(o)}\pi_1 & V_{52}^{(o)}\pi_2 & V_{53}^{(o)} & V_{54}^{(o)}\pi_4 & 1+v_o\pi_5 \end{vmatrix} \div \det\varepsilon \tag{20}$$

where we have used the short notation

$$v_o(q_t, \theta) = V_{11}^{(o)} = V_{22}^{(o)} = V_{33}^{(o)} = V_{44}^{(o)} = V_{55}^{(o)} = \frac{2\pi e^2}{q_t} [P(\theta) + N(\theta)]$$

$$= \frac{2\pi e^2}{q_t} \tanh q_t L [1 + \operatorname{sech} q_t L \cos\theta]^{-1}. \tag{21}$$

Note that $\varepsilon(\theta)$ is a nondiagonal matrix because of which the effective interaction within a given layer j is governed not only by the polarizability function π_j of that layer, but also by the polarizability functions of other layers in the cell. In other words, the effective interaction in a conducting layer is affected, e.g. by excitons in a nearby insulating layer.

For finding the superconducting transition temperature T_c arising from the motion of electrons or holes in a conducting layer j, one has to find the nontrivial solution of the BCS gap equation

$$\Delta_j(\mathbf{k}_t) = -\sum_{\mathbf{k}_t'} V_{jj}(q_t = |\mathbf{k}_t - \mathbf{k}_t'|, \quad \omega = \xi - \xi')\Delta_j(\mathbf{k}_t')$$

$$\times \tanh(\xi'/2k_B T_c)/2\xi', \tag{22}$$

where ξ and ξ' are single-particle energies corresponding to 2-dimensional in-plane wavevectors $\mathbf{k}_t$ and $\mathbf{k}_t'$, respectively, measured from the Fermi-energy of the carriers. As in the case of the usual three-dimensional homogeneous system, the effective interaction $V_{jj}(|\mathbf{k}_t - \mathbf{k}_t'|, \omega)$ can be averaged over the angles between $\mathbf{k}_t$ and $\mathbf{k}_t'$, i.e. equivalent to averaging over q_t for fixed k_t and k_t', since $q_t^2 = k_t^2 + k_t'^2 - 2k_t k_t' \cos\phi$. This implies

$$V_{jj}(q_t, \omega) \to \bar{V}_{jj}(\xi, \xi') = \frac{1}{2\pi} \int_0^{2\pi} d\phi \, V_{jj}(q_t, \omega = \xi - \xi')$$

$$= \frac{2}{\pi} \int_{|k_t - k_t'|}^{k_t + k_t'} dq_t \frac{V_{jj}(q_t, \xi - \xi')}{[2k_t^2 + 2k_t'^2 - q_t^2 - (k_t^2 - k_t'^2)^2/q_t^2]^{1/2}}, \tag{23}$$

so that the energy-dependent BCS gap equation is given by

$$\Delta_j(\xi) = -\int d\xi' \, N_j(\xi') \, \bar{V}_{jj}(\xi, \xi') \, \Delta(\xi') \tanh(\xi'/2k_B T_c)/2\xi' \tag{24}$$

where $N_j(\xi') = d^2 k_t'/4\pi^2 \, d\xi'$ is the 2-dimensional density of states for one type of spin only in the layer j. In the simplest spherical effective mass approximation, $k_t = (k_{Fj}^2 + 2m_j^* \xi/\hbar^2)^{1/2}$, $k_t' = (k_{Fj}^2 + 2m_j^* \xi'/\hbar)^{1/2}$ and $N(\xi') = m_j^*/2\pi\hbar^2$. For k_t and k_t' close to the Fermi surface, (18) can be simplified further to obtain

$$N_j(\xi') \bar{V}_{jj}(\xi, \xi') = N_j \bar{V}_{jj}(\xi - \xi')$$

$$= \frac{m_j^*}{\pi^2 \hbar^2} \int_a^{2k_{Fj}} dq_t \, \frac{V_{jj}(q_t, \omega = \xi - \xi')}{(4k_{Fj}^2 - q_t^2)^{1/2}}, \quad a = \frac{m_j^* |\xi' - \xi|}{\hbar^2 k_{Fj}}. \tag{25}$$

Once, with the use of the solution (19), $V_{jj}(q_t, \omega)$ of (16) is known in the form which can be split into contributions from the exchange of different excitations (phonons, excitons, plasmons, etc.),

$$V_{jj}(q_t, \omega) = \sum_\nu V_{jj}^{(\nu)}(q_t, \omega) \tag{26}$$

having poles at the relevant longitudinal mode frequencies, the usual coupling constants λ_ν, to be used in any superposed square-well model to solve (24) (Srinivasan *et al* 1979), are given by

$$\lambda_\nu \equiv -N_j(o) \, \bar{V}_{jj}^{(\nu)}(o) = -\frac{2N_j(o)}{\pi} \int_0^{2k_{Fj}} dq_t \, \frac{V_{jj}^{(\nu)}(q_t, \omega = 0)}{(4k_{Fj}^2 - q_t^2)^{1/2}} \tag{27}$$

with $N_j = m_j^*/2\pi\hbar^2$ in the spherical effective mass approximation. The usual convention of defining the coupling constants to be positive for attractive interactions has been used. The individual range of these interactions in the square-well model is, of course, determined by the corresponding maximum frequency of the longitudinal excitation for $q_t \sim 2k_{Fj}$ and the Fermi energy E_{Fj} (see Srinivasan *et al* 1979 for defining left and right cut-offs). Of course, if one is willing to solve the gap-equation (24) numerically, with or without the simplification (25), the task of splitting the effective interaction V_{jj} into individual contributions $V_{jj}^{(\nu)}$ of (26) is not necessary. Nevertheless, this splitting and the knowledge of the corresponding coupling constants λ_ν determined by (27) will be extremely useful for understanding the physics of the problem. In what follows, we discuss the next step necessary to tackle the question of finding T_c in layered crystals.

3. Polarization functions of layers and general discussion

In the preceding section, we have obtained an explicit expression for the effective electron–electron interaction in layered crystals, like the new high-T_c oxygen deficient perovskites. The resulting form for the gap-equation for determining T_c due to carriers in a given conducting layer has also been derived. In principle, the calculation of T_c in such quasi-two-dimensional systems by solving this gap equation (24) is straightfor-

ward if we know the polarization functions $\pi_j(q_t, \omega)$ of each of the layers which determine $\bar{V}(\xi - \xi)$ with the use of (16), (19) and (23) or (25). A realistic calculation of π_j, however, requires the knowledge of single-particle electronic band structure states of the carriers in that plane. In the absence of such detailed knowledge at present, in what follows, we can only discuss some extremely simplified forms for these functions, and their possible consequences in determining T_c.

For the electronic part of the polarization, it can be shown that in the limit $\omega \to \infty$, $q_t \to 0$, the intraband "bubble" polarization function in any given two-dimensional conducting layer is given by $-(q_t^2/m^* \omega^2)n_s$, where $n_s = n_c L$ is the surface-density of the carriers in the layer (n_c is the volume carrier density). This implies that in the high frequency limit, $(2\pi e^2/q_t)\pi_c(q_t \to 0, \infty) \to -(\omega_p^2/\omega^2)(q_t L/2)$ for a conducting layer, where $\omega_p = (4\pi n_c e^2/m^*)^{1/2}$ is the usual plasma-frequency parameter of the carriers. Similarly, for $\omega = 0$, $q_t \to 0$, $(2\pi e^2/q_t)$ $\pi_c(q_t \to 0, 0) \to (q_{FT}^2/q_t^2)(q_t L/3)$, where $q_{FT}^2 = 6\pi n_c e^2/E_F$. For interband transitions from a full band to an empty band with a gap frequency ω_g, in the limit $q_t \to 0$, $(2\pi e^2/q_t)\pi^{in} \simeq \omega_v^2(q_t)(q_t L/2)(\omega_g^2(q_t) - \omega^2)^{-1}$, where ω_v is related to an effective "plasma" frequency of the full band. Thus, in a simple approximation, it is possible to take the polarization function for a conducting layer to be of the form

$$\frac{2\pi e^2}{q_t}\pi_j(q_t, \omega) \simeq \frac{\omega_{pj}^2 q_t L/2}{(\frac{1}{2}v_{Fj}^2 q_t^2 - \omega^2)} + \pi_j^{\text{ionic}}(q_t, \omega) \quad \text{[cond. layer]} \qquad (28)$$

where, in terms of the ionic plasma frequency Ω_{pj}^2 the ionic part of the polarization arising from their vibrations in the plane j may be taken to be, $-(\Omega_{pj}^2/\omega^2)(q_t L/2)$. Similarly, for an insulating layer

$$\frac{2\pi e^2}{q_t}\pi_j(q_t, \omega) \simeq \frac{\omega_{vj}^2}{(\omega_g^2 - \omega^2)}(q_t L/2) + \pi_j^{\text{ionic}} \quad \text{[insul. layer]} \qquad (29)$$

Now that we have a preliminary knowledge of the nature of polarization functions, it is possible to examine their consequences in determining the effective interaction $\bar{V}_{jj}$ for a conducting layer and the resulting T_c, by guessing whether in a given crystal, a particular layer is conducting or insulating. However, at this stage of uncertainty in the actual physical parameters of these layered crystals, we would like to resist the usual strong temptation of making an extremely crude calculation of T_c to show that it is in the correct ball-park. A reliable calculation of T_c, even for the usual superconductors, is known to be quite delicate, and we would leave this task to a later publication. However, before closing this paper, what we would like to do is to demonstrate more clearly the fact that electronic excitation in an insulating layer can lead to an additional attractive interaction between carriers in a conducting layer, e.g. in the oxygen deficient C_u-O layers in $YBa_2Cu_3O_{7-\delta}$.

For the purpose of obtaining a physical picture of the effect of insulating layers on a conducting layer, let us assume that only three layers in each unit cell, one central conducting layer with two identical insulating layers on its either side at the same distance d, are important. In other words, let us assume that only significant polarization functions, e.g. are $\pi_3^c(q_t, \omega)$ for the layer 3, which is supposed to be conducting, and $\pi_2^{in}(q_t, \omega) = \pi_4^{in}(q_t, \omega)$ for the insulating layers 2 and 4. Other polarization functions π_0, π_1 and π_5 can be put to zero in (20) for V_{33}, for the sake of

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demonstration only. In such a case, for effective interaction in the conducting layer 3, (20) gives

$$V_{33}(q_t, \omega, \theta) = \det \begin{vmatrix} 1 + v_o\pi_2 & V_{23}^{(o)} & V_{24}^{(o)}\pi_2 \\ V_{32}^{(o)}\pi_2 & V_{33}^{(o)} & V_{34}^{(o)}\pi_2 \\ V_{42}^{(o)}\pi_2 & V_{43}^{(o)} & 1 + v_o\pi_2 \end{vmatrix} \det \begin{vmatrix} 1 + v_o\pi_2 & V_{23}^{(o)}\pi_3 & V_{24}^{(o)}\pi_2 \\ V_{32}^{(o)}\pi_2 & 1 + v_o\pi_3 & V_{34}^{(o)}\pi_2 \\ V_{42}^{(o)}\pi_2 & V_{43}^{(o)}\pi_3 & 1 + v_o\pi_2 \end{vmatrix}^{-1}$$

(30)

where $v_o = V_{22}^{(o)} = V_{33}^{(o)} = V_{44}^{(o)}$ is given by (21) and $V_{32}^{(o)} = V_{43}^{(o)} = V_{23}^{(o)*} = V_{34}^{(o)*}$ and $V_{42}^{(o)*} = V_{24}^{(o)*}$ are obtained from (12) by putting $R_{43} = R_{32} = d$ and $R_{42} = 2d$. The extra interaction $\Delta V_{33}(q_t, \omega, \theta)$ for the carriers in the conducting layer due to the presence of the two insulating layers can then be obtained from the above expression by subtracting from it a term obtained by putting $\pi_2^{in} = 0$ in (30), i.e. subtracting the single-layer interaction term $v_o/(1 + v_o\pi_3^c)$. This, to the lowest order terms in π_2^{in}, leads to

$$\Delta V_{33}(q_t, \omega, \theta) \simeq \frac{-[|V_{32}^{(o)}|^2 + |V_{34}^{(o)}|^2]\,\pi_2^{in}(q_t, \omega)}{[1 + v_o(q_t, \theta)\,\pi_3^c(q_t, \omega)]^2}$$

(31)

Explicitly, one thus gets the desired expression

$$\Delta V_3(q_t, \omega, \theta) = -\frac{2\pi e^2}{q_t}\left[\frac{2\tanh^2 q_t L|\exp(-q_t d) + \exp(i\theta)\sinh q_t d \operatorname{cosech} q_t L|^2}{[1 + (2\pi e^2\pi_3^c/q_t)\tanh q_t L + \operatorname{sech} q_t L\cos\theta]^2}\right]$$
$$\times \left[\frac{2\pi e^2\pi_2^{in}}{q_t}\right].$$

(32)

For a form of $\pi_2^{in}(q_t, \omega)$ similar to (29) for the excitonic part, the above expression gives an attractive interaction for frequencies $\omega < \omega_g$, the longitudinal excitonic (electronic excitation) frequency. Since its range can be much higher than the usual phonon frequencies, even in $YBa_2Cu_3O_{7-\delta}$, this can indeed lead to higher T_c, provided the cut-off factor $\exp(-2q_t d)$, for large interlayer separation, is not very small compared to 1. Since the average interaction $V(\xi - \xi')$ of (25), entering in the superconducting gap equation, is highly weighted towards $q_t = 2k_F$ (much more in our quasi-two-dimensional case than the usual three-dimensional case), it implies that for the maximum impact of well-defined electronic excitations in the insulating layers on T_c for carriers in the conducting layer, $2\,k_F d \sim 1$. For interlayer separation d of the order of 2 Å, this means that k_F should be of the order of about 2×10^7 cm^{-1}, i.e. the layer carrier density $n_s \sim 10^{14}$ cm^{-2}. For low volume carrier densities ($n = n_s/L \sim 10^{21}$ cm^{-3}), reported in the new high-T_c superconductors, this situation seems to be ideal as compared to the case of the usual high-density metals.

It should be emphasized here that the above example of three layers with particular forms of layer polarizabilities was presented only as an illustration. In actual calculation, we hope to include all the relevant layers, with more general forms of polarizabilities which should include the important exchange-correlation effects involving spin-fluctuations (Chaudhury and Jha 1984). Also, we may have to generalize their structure to take into account the role of one-dimensional chains in the layers.

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