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Anisotropy of Gap Parameter in Cuprate Superconductors

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Abstract. — The anisotropy of gap parameter in cuprate superconductors is explained in the frame work of BCS theory using two-dimensional itinerant model of conduction electrons. The BCS gap equation at $T = 0$ is solved in the first iteration approximation. The two-dimensional electron energy bands and electron-phonon interaction in tight-binding approximation are used. The explicit expression for the gap parameter $\Delta^0(\mathbf{k})$ is evaluated for the Einstein model of the solid. It is found that $\Delta^0(\mathbf{k})$ consists of a constant part and an oscillatory part which varies as $\sin^2 k_x a$. The magnitude of oscillatory part is found to depend upon the cutoff energy $\hbar\omega_c$, width of the singularity in the density of states near Fermi surface and overlap integral.

1. Introduction

In the BCS ground state the two electrons of opposite spin and opposite momentum are coupled through the phonon mediated attractive electron-electron interaction [1]. This interaction produces a finite energy gap $\Delta(\mathbf{k})$ at the Fermi surface and the same is given by the integral equation [1]

$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} V_{\mathbf{k}',\mathbf{k}} \left[\Delta(\mathbf{k}')/2E_{\mathbf{k}'}\right] \tanh(E_{\mathbf{k}'}/2k_B T) \tag{1}$$

where $V_{\mathbf{k}',\mathbf{k}}$ is the electron-phonon-electron interaction, $\mathbf{k}' = \mathbf{k} \pm \mathbf{q}$, $\mathbf{q}$ is the phonon wave vector and T is the temperature. $E_{\mathbf{k}}$ is the quasiparticle energy in the superconducting state and is given as $E_{\mathbf{k}} = (\varepsilon_{\mathbf{k}}^2 + \Delta^2(\mathbf{k}))^{1/2}$ where $\varepsilon_{\mathbf{k}}$ is the Bloch energy in the normal state relative to Fermi energy. It was pointed out by Cooper [2] that the form of the integral equation (1) is such that if there is an energy gap over a part of the Fermi surface, there will be one everywhere except perhaps at the isolated points or lines. Thus the nodes were least expected in $\Delta(\mathbf{k})$.

BCS evaluated isotropic gap parameter $\Delta(\mathbf{k}) = \Delta$ for $V_{\mathbf{k}',\mathbf{k}} = -V$ and found that

$$\Delta = 2\hbar\omega_c \exp(-1/n(\varepsilon_f)V) \tag{2}$$

where $\hbar\omega_c$ is the cutoff phonon energy and $n(\varepsilon_f)$ is the electron density of states at the Fermi energy. These authors consistently pointed out that $\Delta(\mathbf{k})$ is anisotropic and many of the transport properties in the superconducting phase may be related to the anisotropic character

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of $\Delta(\mathbf{k})$. However a systematic investigation of anisotropy of $\Delta(\mathbf{k})$ is lacking as most of the later investigations were based on the Eliashberg strong coupling theory [3].

With the invention of high transition temperature T_c in cuprate superconductors [4], the interest in the anisotropy of $\Delta(\mathbf{k})$ is revived to explain high T_c and to understand the nature of BCS ground state [5]. Shen *et al.* [5] attempted to fit their experimental data for $\Delta(\mathbf{k})$ assuming that the BCS ground state has $d_{x^2-y^2}$ symmetry. Mahan [6] fitted the same results assuming the s-symmetry of the BCS ground state. Recently Levi [7] has reviewed the present state of art about the nature of BCS ground state in cuprates.

It was shown by Labbé and Bok [8] and Bok *et al.* [9] that high T_c in cuprates is a consequence of two-dimensional nature of itinerant electrons which are permeated in the periodic square (or rectangular) lattice. Friedel *et al.* have shown [10] that high T_c in A-15 compounds can be explained with the help of tight-binding electron-phonon interaction. This leads us to investigate the anisotropy of $\Delta(\mathbf{k})$ using tight-binding electron energy bands and electron-phonon interaction for a two-dimensional square lattice. We find that $\Delta(\mathbf{k})$ consists of two parts: a constant part and an oscillatory part which varies as $\sin^2 k_x a$ and has the symmetry of a square. This explains the recent results of Shen *et al.* [5].

The plan of the paper is as follows: the necessary formalism is given in Section 2, the calculations and results are presented in Section 3 and these are discussed in Section 4.

2. Theory

It is evident from equation (1) that $\Delta(\mathbf{k})$ will have the symmetry of the eigenvalues of the matrix of elements $V_{\mathbf{k}',\mathbf{k}}$. However, to make the calculations tractable, few approximations have to be made as the self-consistent analytic solution of equation (1) seems improbable. The first approximation we make is that T is nearly zero, therefore $\tanh(E_{\mathbf{k}}/2k_B T) = 1$. This simplifies equation (1) as

$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} V_{\mathbf{k}',\mathbf{k}} \left[\Delta(\mathbf{k}')/(2(\varepsilon_{\mathbf{k}'}^2 + \Delta(\mathbf{k}')^2)^{1/2})\right]. \tag{3}$$

Here all the wave vectors $\mathbf{k}'$ are in the vicinity of Fermi surface (FS) in the range of cutoff phonon energy $\hbar\omega_c$. If $V_{\mathbf{k}',\mathbf{k}}$ is constant, $\Delta(\mathbf{k})$ becomes isotropic, therefore we keep the explicit $(\mathbf{k}',\mathbf{k})$ dependence of $V_{\mathbf{k}',\mathbf{k}}$ and iterate equation (3) for $\Delta(\mathbf{k})$. The first iteration gives

$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} V_{\mathbf{k}',\mathbf{k}} \left[\Delta_0/(2(\varepsilon_{\mathbf{k}'}^2 + \Delta_0^2)^{1/2})\right] \tag{4}$$

where Δ_0 is an initial nonzero gap [1] which is the requirement for a finite T_c.

2.1. Electron Energy Bands. — The strong electron-ion bonding in cuprates occurs in the layers which contain the copper and oxygen ions. Therefore we adopt tight-binding approximation for $\varepsilon_{\mathbf{k}}$ which consists of anisotropic band character. If only the first nearest neighbour overlapping between $d_{x^2-y^2}$ Cu states and $p_{x,y}$ oxygen states is considered, $\varepsilon_{\mathbf{k}}$ in the tetragonal phase is given as [11]

$$\varepsilon_{\mathbf{k}} = \varepsilon_d + (4t_1^2/\varepsilon_0) - (2t_1^2/\varepsilon_0)(\cos k_x a + \cos k_y a) \tag{5}$$

where a is a lattice constant and (k_x, k_y) are the Cartesian components of $\mathbf{k}$. t_1 is the overlap integral between Cu $d_{x^2-y^2}$ and oxygen $p_{x,y}$ states. ε_0 is the splitting between the ionic energies ε_d and ε_p of Cu and oxygen ions respectively. In ionic crystals $t_1 \ll \varepsilon_0$, however, this approximation may not hold very well in high T_c materials.

In this energy band, the electron density is concentrated on the Cu sites. The electrons hop to the adjacent Cu-sites by virtual excitation to the intermediating O-site. This leads to an effective Cu-Cu overlap integral $t = t_1^2/\varepsilon_0$ built up from two consecutive Cu-O-Cu overlaps divided by the excitation energy of the oxygen site. The density of electron states $n(\varepsilon)$ for energy dispersion given in equation (5) contains the van-Hove singularities at the band half width [8] *i.e.*

$$n(\varepsilon) = (N/2\pi^2 D) \ln |D/\varepsilon| \tag{6}$$

where N is the total number of electrons and D is the width of the singularity at the Fermi energy. The singularities arise because the electron group velocity vanishes at the points $\mathbf{k} = [0, \pm\pi/a]$ and $[\pm\pi/a, 0]$ on the square Brillouin zone (BZ). We use equations (5, 6) for $\varepsilon_{\mathbf{k}}$ and $n(\varepsilon)$ respectively in the solution of equation (4).

2.2. Electron-Phonon Interaction. — The superconductivity in cuprates arises due to nonstoichiometry of oxygen. Therefore, both the electrons and holes may contribute in the superconducting process. The exact nature of $V_{\mathbf{k}',\mathbf{k}}$ is expected to be intricate and anisotropic. Therefore we write the model phonon induced electron-electron interaction as [1]

$$V_{\mathbf{k}',\mathbf{k}} = -(V_0 + U_{\mathbf{k}',\mathbf{k}}) \tag{7}$$

where V_0 is a positive constant and $U_{\mathbf{k}',\mathbf{k}}$ explicitly depends upon $\mathbf{k}'$ and $\mathbf{k}$. The magnitude of $V_0 + U_{\mathbf{k}',\mathbf{k}}$ has to be always positive. If $U_{\mathbf{k}',\mathbf{k}}$ is negligibly small, BCS equation (2) for Δ_0 is retrieved. We adopt the electron-phonon interaction suggested by Fröhlich and Mitra [12] to evaluate the anisotropic part $U_{\mathbf{k}',\mathbf{k}}$. In this formalism the electron-phonon matrix element is given as

$$M^{\lambda}_{\mathbf{k}',\mathbf{k}} = -i(q_0/2a)\mathbf{e}^{\lambda}_{\mathbf{k}',\mathbf{k}} \cdot [\mathbf{v}(\mathbf{k}') - \mathbf{v}(\mathbf{k})] + 2i(q_0/a)\mathbf{e}^{\lambda}_{\mathbf{k}',\mathbf{k}} \cdot \mathbf{v}((\mathbf{k}' - \mathbf{k})/2). \tag{8}$$

Here q_0 is the Slater coefficient, $\mathbf{e}^{\lambda}_{\mathbf{q}}$ ($\mathbf{q} = \mathbf{k}' - \mathbf{k}$) is the phonon polarization vector for polarization λ and $\mathbf{v}(\mathbf{k})$ ($= \partial\varepsilon/\partial k$) is the group velocity for the state $|\mathbf{k}\rangle$. The first term of equation (8) is associated with the local variation of the band width in equation (5) and has the major contribution to $M^{\lambda}_{\mathbf{k}',\mathbf{k}}$. The second term of equation (8) arises from the variation of the center of gravity of the band associated with the small variation of the short range Cu-O distances in the second term of equation (5). However the deformation of Cu-O bonds in cuprates are not observed experimentally [13], therefore, the second term of equation (8) is expected to be small. In addition there will be phonon induced variations in ε_{p} and ε_{d} which will lead to an additional electron-phonon interaction which is not explicitly included in equation (8). This term may be important for ionic crystals [14]. In fact it is too difficult to account for $(\mathbf{k}', \mathbf{k})$ dependence of all the contributions to electron-phonon interaction. Therefore we consider here only the explicit $(\mathbf{k}', \mathbf{k})$ dependence of the first term of equation (8) and assume that all other electron-phonon processes, not included in the first term of equation (8), are included in V_0 in equation (7). This simplification may not effectively alter the symmetry of the gap parameter.

The electron-phonon interaction involves the term $(\hbar\omega(\mathbf{q}))^2/[(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'})^2 - (\hbar\omega(\mathbf{q}))^2]$. If $\varepsilon_{\mathbf{k}} = 0$ is the Fermi energy, then the important contribution to $\Delta(\mathbf{k})$ will arise from the states $|\mathbf{k}'\rangle$ near the saddle points taken on the Fermi surface, *i.e.* $\varepsilon_{\mathbf{k}'} \ll \hbar\omega(\mathbf{q})$. With these simplifications $U_{\mathbf{k}',\mathbf{k}}$ is written as

$$U_{\mathbf{k}',\mathbf{k}} = -\sum_{\lambda} |M^{\lambda}_{\mathbf{k}',\mathbf{k}}|^2 / \left[M_{\lambda}\omega^2_{\lambda}(\mathbf{q})\right]. \tag{9}$$

Here M_{λ} is the reduced atomic mass for the vibrational mode λ. In the multiatomic formula unit cell of the cuprates the reduced acoustic and optical masses are different. Considering

the phonon induced change in group velocity $\mathbf{v}(\mathbf{k}') - \mathbf{v}(\mathbf{k})$ along the direction of phonon propagation and using equation (8) in (9) we get

$$U_{\mathbf{k}',\mathbf{k}} = -(q_0^2/4a^2)|\left[\mathbf{v}(\mathbf{k}') - \mathbf{v}(\mathbf{k})\right]|^2 \sum_\lambda |\mathbf{e}_\mathbf{q}^\lambda|^2 / \left[M_\lambda \omega_\lambda^2(\mathbf{q})\right]. \tag{10}$$

From equation (8) we find that as $q \to 0$, $M_{\mathbf{k}',\mathbf{k}}^\lambda \to 0$. Therefore to keep $U_{\mathbf{k}',\mathbf{k}}$ finite, small values of $\omega_\lambda(\mathbf{q})$ must be accounted for. In other words the contribution of acoustic phonons which modulate locally the Cu-Cu distances in the conducting plane should be included. However the compensation between $M_{\mathbf{k}',\mathbf{k}}^\lambda$ and $\omega_\lambda(\mathbf{q})$ for small values of $\mathbf{q}$ can be completed in two ways. First the phonons with very small values of frequencies are eliminated from superconductivity by the inequality $\hbar\omega(\mathbf{q}) \gg |\varepsilon_{\mathbf{k}'} - \varepsilon_\mathbf{k}|$. Therefore acoustic modes can be treated more like the Einstein modes. Secondly the $\mathbf{q}$ in $M_{\mathbf{k}',\mathbf{k}}^\lambda$ is a two-dimensional vector while in $\omega_\lambda(\mathbf{q})$ it is three-dimensional because the material has the isotropic elastic properties. The large components of $\mathbf{q}$ perpendicular to the conducting plane make $\omega_\lambda(\mathbf{q})$ large.

The neutron and Raman scattering experiments [15] show that the cuprates consist of large number of optical phonons and these are about ten times more energetic than the acoustic phonons. In view of these facts we assume all the acoustic and optical phonons as the degenerate Einstein modes. This simplifies the last factor of equation (10) as

$$\sum_\lambda |\mathbf{e}_\mathbf{q}^\lambda|^2 / \left[M_\lambda \omega_\lambda^2(\mathbf{q})\right] = n_\mathrm{E}/M_\mathrm{E}\omega_\mathrm{o}^2 \tag{11}$$

where n_E is the number of Einstein modes, ω_o is the Einstein frequency and M_E is the reduced Einstein mass. If there is one copper atom and two oxygen atoms in the unit cell of square lattice $M_\mathrm{E} = (M_\mathrm{c}M_\mathrm{x})/\left[2M_\mathrm{c} + M_\mathrm{x}\right]$ for the optical Einstein modes where M_c and M_x are the copper and oxygen atomic masses respectively. The longitudinal and transverse modes are degenerate at the zone boundary along the [11] direction. In obtaining equation (10) the coupling of the electrons with the phonons in the z-direction is partially included, which will be discussed later.

2.3. Evaluation of Equation (4). — Using the above simplifications in equation (4), we get

$$\Delta(\mathbf{k}) = \Delta_1 - \Delta_2(\mathbf{k}) \tag{12}$$

where

$$\Delta_1 = (V_0\Delta_0/2) \sum_{\mathbf{k}'} \frac{1}{\sqrt{\varepsilon_{\mathbf{k}'}^2 + \Delta_0^2}} \tag{13}$$

and

$$\Delta_2(\mathbf{k}) = \left[(q_0^2\Delta_0 n_\mathrm{E})/(4a^2 M_\mathrm{E}\omega_0^2)\right] \sum_{\mathbf{k}'} \frac{|\left[\mathbf{v}(\mathbf{k}') - \mathbf{v}(\mathbf{k})\right]|^2}{(1/2)(1/(\varepsilon_{\mathbf{k}'}^2 + \Delta_0^2)^{1/2})}. \tag{14}$$

Considering the spin degeneracy factor and replacing the sum over $\mathbf{k}'$ by integration in the two-dimensional BZ, equations (13, 14) simplify as

$$\Delta_1 = (V_0\Delta_0/2)\frac{A}{2\pi^2} \int\int \frac{\mathrm{d}\mathbf{k}'}{\sqrt{\varepsilon_{\mathbf{k}'}^2 + \Delta_0^2}} \tag{15}$$

and

$$\Delta_2(\mathbf{k}) = \left[(q_0^2\Delta_0 n_\mathrm{E})/(4a^2 M_\mathrm{E}\omega_0^2)\right] \left[A/(2\pi)^2\right] \int\int \mathrm{d}\mathbf{k}' \frac{|\mathbf{v}(\mathbf{k}') - \mathbf{v}(\mathbf{k})|^2}{\sqrt{\varepsilon_{\mathbf{k}'}^2 + \Delta_0^2}} \tag{16}$$

where A is the area of the square lattice. The integration over $\mathbf{k}'$ is to be carried out in the vicinity of Fermi energy such that $\varepsilon_{\mathbf{k}'} < \hbar\omega_c$ as discussed by BCS [1].
To facilitate the integrations in equations (15, 16) we write

$$\mathrm{d}\mathbf{k}' = \mathrm{d}k'_\perp \mathrm{d}k'_t = (\mathrm{d}k'_\perp/\mathrm{d}\varepsilon)\mathrm{d}\varepsilon\mathrm{d}k'_t = \mathrm{d}\varepsilon\mathrm{d}k'_t/|\mathbf{v}'_g| \tag{17}$$

where $\mathbf{v}'_g = \mathbf{v}(\mathbf{k}')$ and k'_t and $k'_\perp$ are the rectangular components of $\mathbf{k}'$ along the tangent and normal to the edge of the square Fermi surface respectively. Using equation (17) in (15) and (16) we get

$$\Delta_1 = (V_0\Delta_0/2)\int_0^{\hbar\omega_c} \frac{n(\varepsilon)\mathrm{d}\varepsilon}{\sqrt{\varepsilon^2+\Delta_0^2}} \tag{18}$$

and

$$\begin{aligned}\Delta_2(\mathbf{k}) &= \left[(q_0^2\Delta_0 n_E)/(4a^2M_E\omega_0^2)\right]\left[A/(2\pi)^2\right]\int_0^{\hbar\omega_c}\frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon^2+\Delta_0^2}} \\ &\times \oint \frac{\mathrm{d}k'_t}{|\mathbf{v}'_g|}\left[|\mathbf{v}'_g|^2+|\mathbf{v}(\mathbf{k})|^2-2\mathbf{v}'_g\ \ \mathbf{v}(\mathbf{k})\right].\end{aligned} \tag{19}$$

The integral over $\mathrm{d}k'_t$ is along the edges of the Fermi square and $n(\varepsilon)$ is defined as [9]

$$n(\varepsilon) = \left[A/(2\pi^2)\right]\oint\frac{\mathrm{d}k'_t}{|\mathbf{v}'_g|}\cdot \tag{20}$$

The last term of equation (19) vanishes due to symmetry. Use of equation (20) in (19) gives

$$\begin{aligned}\Delta_2(\mathbf{k}) &= \left[(q_0^2\Delta_0 n_E)/(4a^2M_E\omega_0^2)\right]\left[(A/(2\pi)^2)\int_0^{\hbar\omega_c}\frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon^2+\Delta_0^2}}\oint|\mathbf{v}'_g|\mathrm{d}k'_t\right. \\ &\left.+(1/2)|\mathbf{v}(\mathbf{k})|^2\int_0^{\hbar\omega_c}\frac{n(\varepsilon)\mathrm{d}\varepsilon}{\sqrt{\varepsilon^2+\Delta_0^2}}\right].\end{aligned} \tag{21}$$

Using the relations

$$\begin{aligned}|\mathbf{v}'_g| &= 2\sqrt{2}|t|a|\sin k_x a| \\ k_x &= k_t/\sqrt{2} \\ \oint|\mathbf{v}'_g|\mathrm{d}k_t &= 32|t|\end{aligned} \tag{22}$$

equation (21) simplifies as

$$\begin{aligned}\Delta_2(\mathbf{k}) &= \left[(q_0^2\Delta_0 n_E)/(4a^2M_E\omega_0^2)\right]\left[\frac{A\ 32|t|}{(2\pi)^2}\ln\left(\hbar\omega_c/\Delta_0\right.\right. \\ &\left.\left.+\sqrt{(\hbar\omega_c/\Delta_0)^2+1}\right)+(1/2)|\mathbf{v}(\mathbf{k})|^2\int_0^{\hbar\omega_c}\frac{n(\varepsilon)\mathrm{d}\varepsilon}{\sqrt{\varepsilon_0^2+\Delta^2}}\right].\end{aligned} \tag{23}$$

Evidently Δ_1 depends on V_0, cutoff energy $\hbar\omega_c$ and the density of states $n(\varepsilon)$ as found in BCS theory. In addition $\Delta_2(\mathbf{k})$ also depends on the screening length q_0, Einstein phonon energy $a^2M_E\omega_0^2$ and the reduced overlap integral t. In this simplified but realistic physical model the anisotropy of $\Delta(\mathbf{k})$ is the same as that of $\Delta_2(\mathbf{k})$ which varies as $|\mathbf{v}(\mathbf{k})|^2$.

Labbé and Bok [8,9] calculated density of states for a rectangular lattice in the tight-binding approximation and expressed equation (6) as

$$\begin{aligned} n(\varepsilon) &= n_0 + n_1 \ln|D/\varepsilon|; \quad -D < \varepsilon < D \\ &= n_0 \qquad\qquad\qquad\qquad \varepsilon \in [-W/2, -D] \cup [D, W/2] \end{aligned} \tag{24}$$

where $n_0 = 1/(4\pi|t|)$ per copper atom, $n_1 = 1/2\pi^2 D$ per copper atom and W is the band width. Since $\hbar\omega_c < D$, the first equality of equation (24) is used in the calculations of equations (18, 23). n_0 and n_1 are determined by the condition $n_0 W + 2n_1 D = 1$ and

$$\begin{aligned} |\mathbf{v}(\mathbf{k})|^2 &= 4a^2t^2(\sin^2 k_x a + \sin^2 k_y a) \\ &= 8a^2t^2 \sin^2 k_x a \end{aligned} \tag{25}$$

because $k_y = \pi/a \pm k_x$ at the square Fermi surface. Equations (24, 25) are used in equations (18, 23) to evaluate the gap parameter per copper atom which is written as

$$\Delta(\mathbf{k}) = C_1 - C_2|\sin k_x a|^2 \tag{26}$$

where

$$C_1 = (V_0\Delta_0/2)\,[n_0 f_1 + n_1 f_2] - C_0 \frac{32|t|}{(2\pi)^2} f_1, \tag{27a}$$

$$C_2 = C_0(4t^2)\,[n_0 f_1 + n_1 f_2], \tag{27b}$$

$$f_1 = \ln\left[(\hbar\omega_c/\Delta_0) + \sqrt{(\hbar\omega_c/\Delta_0)^2 + 1}\right], \tag{27c}$$

$$f_2 = \int_0^{\hbar\omega_c} \frac{\ln|D/\varepsilon|}{\sqrt{\varepsilon^2 + \Delta_0^2}} \mathrm{d}\varepsilon, \tag{27d}$$

and

$$C_0 = (q_0 a)^2 n_E/(4a^2 M_E \omega_0^2/\Delta_0). \tag{27e}$$

Here C_1 has to be always greater than C_2 so that $V_{\mathbf{k}',\mathbf{k}}$, given in equation (7), is negative. The important feature of equation (26) is that $\Delta(\mathbf{k})$ consists of two parts: a constant part and an oscillatory part varying as $\sin^2 k_x a$, which has the four fold rotation symmetry of the square lattice. Since the two contributions are of the opposite sign, $|\Delta(\mathbf{k})|$ will be maximum in the vicinity of the van-Hove points and minimum in the middle of the two van-Hove points. This is essentially observed by Shen *et al.* [5] by angular photoemission experiments in the *ab* plane of $Bi_2Sr_2CaCu_2O_{8+\delta}$. Since $C_1 > C_2$, there should always be a gap, howsoever small it may be. In the following we present the model calculations for $\Delta(\mathbf{k})$.

3. Calculations and Results

The observed energy gap parameter $\Delta^0(\mathbf{k})$ for a superconductor is given as

$$\begin{aligned} \Delta^0(\mathbf{k}) &= 2|\Delta(\mathbf{k})| \\ &= 2|C_1 - C_2 \sin^2 k_x a|. \end{aligned} \tag{28}$$

From equation (28)

$$\Delta^0_{\mathrm{mx}} = 2|C_1|; \qquad k_x = 0 \tag{29a}$$

and

$$\Delta^0_{\mathrm{mi}} = 2|C_1 - C_2|; \qquad k_x = \pi/2a. \tag{29b}$$

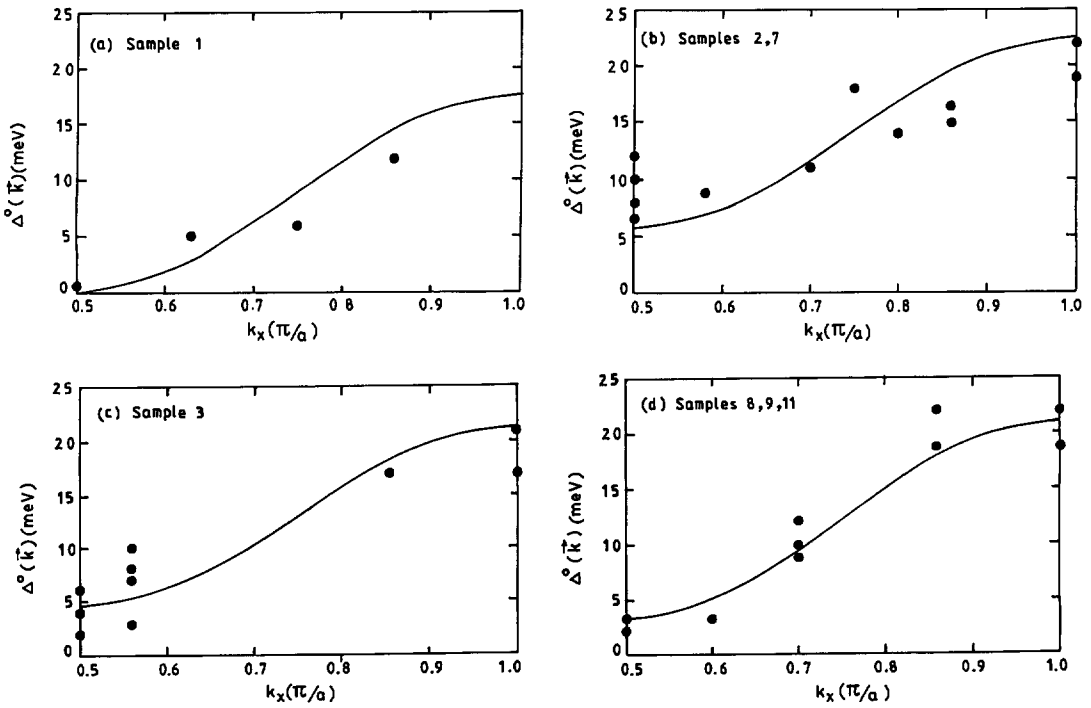

Fig. 1. — $\Delta^0(\mathbf{k})$ *versus* (k_x, k_y). The solid circles are the experimental points and the solid lines are the results of equation (28): (a) sample #1; (b) samples #2, 7; (c) sample #3; (d) samples # 8, 9, 11. The k_y coordinate is $-k_x + (\pi/a)$.

Here $\Delta^0_{\rm mx}$ and $\Delta^0_{\rm mi}$ are the maximum and minimum gaps at the van-Hove points and between the two van-Hove points respectively. For a quantitative explanation of the experimental data of Shen *et al.* we have taken $q_0 a \simeq 1$ assuming that the d-wave inverse screening length is of the order of a^{-1} For a square lattice of Cu-O plane $n_{\rm E} = 4$. The initial gap parameter Δ_0 should be of the order of average optical phonon energy, therefore we choose $a^2 M_{\rm E}\omega_0^2/\Delta_0 = 1$. With these simplifications $C_0 = 1$ (Eq. (27e)). Substituting n_0 and n_1, one finds

$$C_1 = V_0\Delta_0\,[0.04\ f_1/|t| + 0.025\ f_2/|D|] - 0.81\ f_1|t|$$

and

$$C_2 = t^2\,[0.32\ f_1/|t| + 0.20\ f_2/|D|]\,.$$

The overlap integral t_1 has been estimated from band structure calculations [16] and experimental measurements [17, 18]. From experimental measurements t_1 is found between 0.20 to 0.25 eV. Here in our calculations $t = t_1^2/\varepsilon_0$ is the reduced Cu-O-Cu overlap integral, therefore we keep $t = 0.01$ eV [11] and determine the parameter D by the relation $D = 16t$ [9]. The optical phonon energy varies from 20 meV to 100 meV. We take average optical phonon energy $\hbar\omega_{\rm c} = 60$ meV. With this reasonable set of parameters we calculated $\Delta^0(\mathbf{k})$ *versus* $\mathbf{k}$. We varied the constant part of electron-phonon interaction V_0 and the initial gap parameter Δ_0 such that $C_1 > C_2$ always. The calculated results are compared with experimental data in Figure 1. The experimental data is on the Fermi line which is along the [11] direction. Shen *et al.* have shown $\Delta^0(\mathbf{k})$ *versus* $0.5|\cos k_x a - \cos k_y a| = |\cos k_x a|$ on the Fermi surface. We have rewritten their data on the (k_x, k_y) scale. Although there are large error bars in the experimental data

Table I. — *The initial parameters and calculated results for $\Delta^0(\mathbf{k})$ for different samples. Δ_0 is the initial gap parameter, V_0 is the constant part of electron-phonon interaction and (C_1, C_2) are the calculated parameters as defined in the text. $\Delta^0_{\rm mx}$ and $\Delta^0_{\rm mi}$ are the maximum and minimum gaps respectively. All the quantities are in meV. In these calculations $q_0 a = 1$, $a^2 M_0 \omega_0^2/\Delta_0 = 1$, reduced overlap integral $t = 10$ meV, width of singularity $D = 16t$ and cutoff energy $\hbar\omega_{\rm c} = 60$ meV are used.*

samples	Δ_0	V_0	C_1	C_2	$\Delta^0_{\rm mx}$	$\Delta^0_{\rm mi}$	$\Delta^0_{\rm mx}/\Delta^0_{\rm mi}$
1	10	265	8.86	8.76	17.71	0.18	98.39
2, 7	11	265	11.30	8.40	22.56	5.71	3.95
3	11	260	10.69	8.40	21.37	4.58	4.67
8, 9, 11	10	280	10.50	8.80	21.00	3.47	6.05

and there are many simplifications in the theory too, the calculated results represent very well the experimental data. The ratio $\Delta^0_{\rm mx}/\Delta^0_{\rm mi}$ varies from 4 to 100 for different samples. The input parameters and calculated results are tabulated in Table I. It is found that by increasing $\hbar\omega_{\rm c}$, $\Delta^0(\mathbf{k})$ is enhanced, however its general behaviour remains the same.

The overlap parameter t is important in determining the itinerant character of charge carriers. Here t depends upon t_1 and ε_0 and t_1 is sensitive to inverse screening length q_0. Therefore we varied t from 0.01 to 0.15 eV. It is found that by making the corresponding changes in the values of $q_0 a$ from 1 to 0.08 and adjusting the value of V_0 such that $C_1 > C_2$, the results remain similar to those given in Figure 1. There is a closeness in the values of C_1 and C_2 in Table I. This indicates that both Δ_1 and Δ_2 in equation (12) arise from the electron-phonon coupling of the same physical origin. These two contributions compensate each other, therefore, it can argued that C_1 and C_2 arise due to phonon induced electron-electron attraction and electron-hole repulsion respectively. We also calculated $\Delta^0(\mathbf{k})$ as the function of ϕ which is the angle of $\mathbf{k}$ with respect to k_x axis in the (k_x, k_y) plane. In this representation equation (28) becomes

$$\Delta^0(\phi) = 2|C_1 - C_2 \sin^2(\pi/(1+\tan\phi))| \tag{30}$$

where $\tan\phi = k_y/k_x$ and $0 < \phi < \pi/2$ on the square Fermi surface. Evidently the gap is maximum for $\phi = 0$ and minimum for $\phi = \pi/4$. The results of equation (30) can also be compared with the experimental data rewritten on the scale $\tan\phi = k_y/k_x$. A schematic representation of $\Delta^0(\phi)$ with four fold rotation symmetry of the square in the (k_x, k_y) plane is shown in Figure 2.

4. Discussion

Assuming that the cuprates are d-wave superconductors, Shen *et al.* [5] expressed the gap parameter for a square lattice as:

$$\Delta^0_{\rm d}(\mathbf{k}) = \Delta_{\rm d0}|\cos k_x a - \cos k_y a|. \tag{31}$$

The photoemission measurements give $|\Delta^0_{\rm d}(\phi)|$. Therefore Shen *et al.* attempted to fit their data by the straight line $|\Delta^0_{\rm d}(\phi)|$ *versus* $|\cos k_x a|$. In equation (31) the gap varies from 0 to $2\Delta_{\rm d0}$ on the Fermi surface. However the question is: can the zero gap be measured within the experimental accuracies. Mahan [6] has shown that the data of Shen *et al.* can be fitted with the s-wave order parameter which, in the lowest order for a square lattice, is given as:

$$\Delta^0_{\rm s}(\phi) = \Delta_{\rm n} + \Delta_4 \cos(4\phi) \tag{32}$$

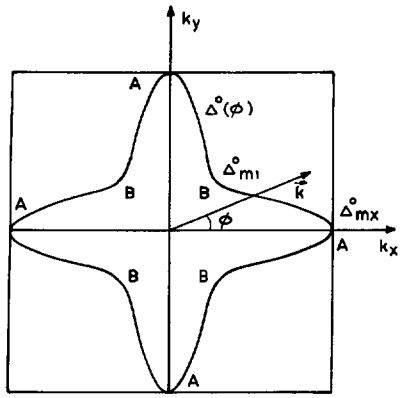

Fig. 2. — Schematic variation of $\Delta^0(\phi)$ in the (k_x, k_y) plane along the square Fermi surface. The gap is maximum at the van-Hove points A ($\phi = 0$) and minimum between the van-Hove points B ($\phi = \pi/4$). $\Delta^0(\phi)$ has the four fold rotation symmetry of the square.

where Δ_n and Δ_4 are constants. Recently Kirtley *et al.* [19] reported the direct experimental observations of spontaneous magnetization at a tricrystal point in a polycrystalline thin film of Y-123. The tricrystal geometry produces an odd number of negative Josephson critical currents around a path enclosing the tricrystal point if the order parameter of Y-123 has d-wave symmetry. However these authors have pointed out that their modeling of tricrystal vortex could be inaccurate because the magnetic fields inside the grain boundary are modeled assuming an infinitely thick film.

In the present model of electron-phonon interaction, we can rewrite equation (28) as

$$\Delta^0(\mathbf{k}) = \Delta^0_{\mathrm{mi}} + 2C_2(\cos k_x a)^2. \tag{33}$$

Thus $\Delta^0(\mathbf{k})$ *versus* $\cos k_x a$ will be a parabola with an intercept Δ^0_{mi}. This is the trend of data points for samples 1, 2, 3, 5, 7, 8, 9 and 11 where the data points are more than three. We can also rewrite equation (33) as:

$$\Delta^0(\phi) = (\Delta^0_{\mathrm{mi}} - C_2) + C_2 \cos(2\pi/(1 + \tan\phi)). \tag{34}$$

Thus $\Delta^0(\phi)$ *versus* $\cos(2\pi/(1 + \tan\phi))$ will be a straight line with a finite intercept.

Thus Shen *et al.* [5] and Kritly *et al.* [19] have attempted to interpret their results assuming that the gap parameter $\Delta^0(\mathbf{k})$ has d-wave symmetry. However it is shown in the present calculations that the data of Shen *et al.* can equally be explained using anisotropic electron-phonon interaction. There may be other ways to explain the experimental data also but at this juncture the possibility of electron-phonon coupling being the origin of such a gap is not ruled out. However much work is needed to understand the electron-phonon interaction in cuprates.

In the present calculations, we have used the energy band structure and the electron-phonon interaction for the two-dimensional square lattice to explain the anisotropy of gap parameter. In the energy bands only the first nearest neighbour interaction is considered. Addition of the second nearest neighbour interaction may account for the deviation of FS from an exact square and hence may further contribute to the anisotropy of gap parameter. Further the electron-phonon interaction is calculated in the linear approximation. The non-linear terms will also contribute towards the anisotropic character of $\Delta^0(\mathbf{k})$. It is expected that these contributions may be corrections to $\Delta^0(\mathbf{k})$ and the essential features will remain the same.

In the present calculations, the electron-phonon coupling in the z-direction is implicitly included. It has been shown by Fortini [20] that this coupling brings in the effect of apical oxygen which has been found important in the explanation of higher T_c. The detailed calculations of the second term of equation (8) give the small oscillatory contribution to $\Delta^0(\mathbf{k})$. Thus the second term of equation (26) will be enhanced. However the general characteristics remain the same. These calculations along with temperature dependence of $\Delta^0(\mathbf{k})$ will be reported later.

There are many questions yet to be answered. However the most important conclusion has been that even the first order iteration of BCS integral equation for $\Delta^0(\mathbf{k})$ near $T = 0$ gives the required symmetry of $\Delta^0(\mathbf{k})$ with the help of well established electron-phonon interaction. This shows that the BCS prescriptions for nearly two-dimensional system may continue to explain the high T_c in cuprates.

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