Electron-phonon interaction near Van Hove singularities

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The Eliashberg equations are solved in two dimensions for the transition temperature of a superconductor. The density of states has a logarithmic singularity. We show that the singularity in the density of states has only a small influence on the numerical solutions to the Eliashberg equations, apart from its contributions to the electron-phonon interaction λ . We also consider the effects of the angular dependence of the gap around the Fermi line which occur for s-wave pairing.

I. INTRODUCTION

Eliashberg¹ equations describe superconductivity in metals where the electron-phonon interactions cause the pair binding. They are often solved to describe superconductivity in three-dimensional metals.²⁻⁶ In the high-temperature superconductors the conduction electrons are confined to planes, and their motion is largely two dimensional. Here we solve the Eliashberg equations for a two-dimensional metal.

In two dimensions the density of states⁷ of the electrons has a Van Hove singularity which goes as $\rho(E) \sim -\ln|E - E_s|$, where the singularity is at an energy E_s . The present calculations were undertaken to investigate whether this singularity, in the density of states, has an important effect on the solutions to the Eliashberg equations. In particular, we focus on the calculation of the transition temperature T_c of the superconductor. We note, in passing, that many papers $^{8-11}$ have been written on electronic mechanisms for high T_c due to Van Hove singularities. Also, many papers were written on the A-15 compounds regarding the relationship between super-conductivity and the density of states.¹²⁻¹⁴ This started with Horsch and Rietschel¹² and is reviewed in Ref. 5. This work was in three dimensions, where there is no logarithmic singularity. The present work is the first to solve the Eliashberg equations for a logarithmic singularity in the density of states.

In three dimensions, most metals have the density of states of the electron being a smooth function of the energy. Then T_c is determined by two-dimensionless parameters: λ is the strength of the attractive electron-phonon interaction, while μ^* is the relative strength of the repulsive electron-electron interactions. The latter constant seems to have a universal value around $\mu^*=0.1$. There is also a dimensional constant in the average phonon energy. If superconductivity is caused by the electron-phonon interaction, then T_c increases with increasing values of λ .

Whether or not high-temperature superconductivity in cuprates is caused by the electron-phonon interaction is a topic of considerable debate.¹⁵⁻¹⁸ Numerous other mechanisms have been proposed.¹⁹⁻²⁴ Here we make no claim to decide which mechanism is operating. Instead,

we are only examining the electron-phonon mechanism in two dimensions, so see whether there are significant differences from three dimensions.

In two dimensions our theory has only four parameters: λ , μ^* , the chemical potential μ , and the average phonon energy. The chemical potential enters only through its energy separation from the singularity energy $E_{\rm s}$. Superconductivity is caused by the pairing of electrons at the chemical potential, which makes this the important energy for electrons. We find that if $|\mu - E_s|$ is more than 10% of the bandwidth, then the singularity has no effect. The exact definition of "no effect" is given below. However, we divide the effects of the singularity into two categories: one is the effect on λ while the other is just due to small values of $|\mu - E_s|$, and how that affects the solution to the equations. The latter category is the main one we investigate. Cuprate superconductors must be alloyed in order to become superconductors, so that the chemical potential is not too near the singular energy. So our conclusion is that the singularity in two dimensions does not help the onset of superconductivity, and does not explain high-temperature superconductivity. A separate question is the effect of the singularity on λ . That is a more subtle question which is also discussed.

We also consider how the energy gap of the superconductor depends upon angle around the Fermi line in two dimensions. In three dimensions, Fermi-surface anisotropy can make the gap anisotropic.²⁵⁻²⁷ We assume s-wave pairing, and that the x and y directions are equivalent. Then the gap can be expanded in a set of functions called "Fermi-surface harmonics" (FSH).³⁻⁵ Many such functions have been used. Previously we introduced²⁸ a set of FSH of the form $cos(4l\phi)$ where l is an integer

$$\Delta(\phi) = \sum_{l} \Delta_{4l} \cos(4l\phi) . \tag{1}$$

An isotropic gap would have only the first term on the right. We examine whether the $\cos(4\phi)$ term significantly changes the transition temperature of the superconductor. We find that it does in certain cases. Earlier we discussed how this kind of angular dependence affected the density of states observed in electron tunneling.

Recently there has been experimental $evidence^{29-31}$ which suggests that the gap could have *d*-wave symme-

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try. We show that the photoemission data can be explained equally well by the present theory using s-wave symmetry.

II. ISOTROPIC EQUATIONS

In two dimensions the electron has a dispersion relation E_k . An important function in the theory is the density of states $\rho(\omega)$ which is defined for a single-spin state as

$$\rho(\omega) = \int \frac{d^2k}{(2\pi)^2} \delta(\omega - E_k) . \qquad (2)$$

In high-temperature superconductors the conduction electrons are in a plane of copper and oxygen atoms. The electron motion is described by tight-binding models, where the electron hops between neighboring orbitals.⁷

In the present calculations, we took the simplest tightbinding model for two dimensions. It is a square lattice of constant *a* with identical *s* orbitals on each site. The hopping energy is *t* and the bandwidth is 8*t*. It is convenient to normalize all energies to 4*t*, so that the electron energy is $v=\omega/4t$ and the chemical potential is $u=\mu/4t$. For this model the density of states is well known to be given by an elliptic integral

$$E_{\mathbf{k}} = -2t(\cos\theta_x + \cos\theta_y) , \qquad (3)$$

$$\theta_{\mu} = k_{\mu}a \quad , \tag{4}$$

$$\rho(\omega) = \frac{1}{4\pi t a^2} h(v) , \qquad (5)$$

$$h(v) = \frac{2}{\pi} K(1 - v^2) .$$
 (6)

The dimensionless factor h(v) in the density of states is $h(\pm 1)=1$ at the end points, and diverges logarithmically as $|u| \rightarrow 0 = E_s$. This factor plays a key role in the theory. Any tight-binding model in two dimensions has a similar divergence. The present model has the advantage of being easy to program. The divergence is the interesting aspect of the calculation. How does it affect the solution to the equations for superconductivity? Our conclusions will apply to any model which has such a divergence, which, in fact, is almost any model.

The self-energy of the electron, from its interaction with phonons, is given by the usual expression⁶

$$\Sigma(\mathbf{k}, ip_n) = \sum_{\nu} \int \frac{d^3 q}{(2\pi)^3} |M_{\nu}(\mathbf{k}, \mathbf{k} + \mathbf{q})|^2 \\ \times \left[\frac{n_B[\omega_{\nu}(\mathbf{q})] + 1 - n_F(E_{k+q})}{ip_n + \mu - E_{k+q} - \omega_{\nu}(\mathbf{q})} + \frac{n_B[\omega_{\nu}(\mathbf{q})] + n_F(E_{k+q})}{ip_n + \mu - E_{k+q} + \omega_{\nu}(\mathbf{q})} \right].$$
(7)

We are using the formalism for nonzero temperature, where the self-energies are expressed in energies $p_n = 2\pi k_B T(n + \frac{1}{2})$. The matrix element M_v has been screened by the electron-electron interaction. The summation v is over the different polarization modes of the phonon system.

We decided to adopt a simple model for the phonon system. It has an Einstein spectrum: there is only one phonon energy ω_0 and the matrix element M_v is a constant M_0 . In this model the strength of the electronphonon coupling is given by the dimensionless parameter λ which is

$$\lambda = \frac{2M_0^2}{c\omega_0} \frac{h(u)}{4\pi t a^2} , \qquad (8)$$

$$\Sigma(ip_n) = 4t\sigma_n$$
,

$$\Gamma_{n} = \frac{\lambda v_{0}}{2} \int_{-1}^{-1} dv g(v) \left[\frac{N_{0} + 1 - n_{F}(v)}{id(n + \frac{1}{2}) + u - v - v_{0}} + \frac{N_{0} + n_{F}(v)}{id(n + \frac{1}{2}) + u - v + v_{0}} \right], \quad (10)$$

$$g(v) = \frac{h(v)}{h(u)} , \qquad (11)$$

$$d = \frac{2\pi k_B T}{4t} , \qquad (12)$$

$$v_0 = \omega_0 / 4t , \qquad (13)$$

$$N_0 = \frac{1}{\exp(2\pi\nu_0/d) - 1}$$
 (14)

The parameter c is the lattice spacing perpendicular to the plane. The self-energy of the electron Σ_n depends only upon the integer n as well as the temperature and chemical potential $\mu = 4tu$. The density-of-states factor h(v) enters several places: in $\lambda \propto h(u)$, in the screening of the matrix element, and also in the density of electron states in the integration. The factor g(v) is the relative density of states, compared to the value at the chemical potential. The interesting question is which factor is the most important. We will show that the answer is that λ is most important. The factor of g(v) has almost no effect unless u is within 10% of the singular energy.

The second equation determines the transition temperature of a superconductor. At this temperature T_c the Eliashberg equations become a linear equation for the correlation function W(p) which gives the pairing in the superconducting state. In a four-vector notation it is

$$W(p) = \int dk \, \mathcal{V}(p,k) \frac{W(k)}{|ik + \mu - E_k - \Sigma(k)|^2} \,. \tag{15}$$

The factor $\mathcal{V}(p,k)$ is the effective interaction between the electrons. The phonon part of this is rather simple in our present model of Einstein phonons and constant matrix element. There is also a small repulsive contribution from electron-electron interactions. This latter term introduces a parameter μ^* into the Eliashberg equations. We omit any influence of impurities.

With these approximations, the above equation simplifies to⁵

$$W_n = \sum_m \left[\frac{\lambda f_m}{1 + b^2 (n - m)^2} - \mu^* \right] W_m ,$$
 (16)

(9)

$$b = \frac{2\pi k_B T}{\hbar\omega_0} , \qquad (17)$$

$$f_m = \frac{d}{2\pi} \int_{-1}^{1} dv \frac{g(v)}{|id(m + \frac{1}{2}) + u - v - \sigma_m|^2} .$$
(18)

The Eliashberg equation is (16). One chooses the parameters λ , μ , T. One evaluates the self-energy in (10) and then the other integral in (18). One evaluates the determinant implied by (16). The temperature is varied until this determinant vanishes. Then one has found T_c for these values of λ and u. The solution of these equations are well known when the density of states h(v) is smooth.

For electron motion in two dimensions, the density of states always has a logarithmic singularity at some energy near the middle of the band. The question of interest is whether this singularity has a large effect on the transition temperature of a superconductor. In the present model the density of states enters two places in the equations: it affects the electron-phonon coupling strength λ and also enters into the relative density of states g(v). We treat these two factors separately.

First consider the factor g(v). It is the density of states of an electron of energy v divided by the density of states at the chemical potential. It enters into the integral (10) for the self-energy and also into the integral (18) for f_m . In cases where the density of states is smooth, then g(v)equals one everywhere. In that case, and when the bandwidth is unlimited, the integral in (18) gives

$$f_m = \frac{1}{|(2m+1)Z_m|} , \qquad (19)$$

$$Z_m = 1 - \frac{\sigma_m}{id(m + \frac{1}{2})} .$$
 (20)

The factor $Z_0 = 1 + \lambda$ but Z_m decreases to unity for larger values of *m*. In this case the solution to (16) gives a wellknown curve of T_c / ω_0 vs λ . Figure 1 shows this curve as the solid line for $\mu^* = 0.1$ and $\omega_0 = 0.05$ eV which agrees with the standard curve in Ref. 5. If one omits the



FIG. 1. The superconducting transition temperature T_c as a function of coupling constant λ for the case that $\mu^*=0.1$ (solid line) and $\mu^*=0$ (dashed line). The phonon frequency is $\omega_0=0.05$ eV.



FIG. 2. T_c as a function of chemical potential for $\lambda = 1.25$ and $\omega_0 = 0.05$ eV ($\nu_0 = 0.0125$). The Van Hove singularity is at E = 0 and the chemical potential is normalized to give u = -1at the bottom of the band and u = 0 at the singularity. T_c is affected mostly within 10% of the singular energy.

Coulomb repulsion $\mu^*=0$, then one gets the dotted line in Fig. 1.

From now on we omit μ^* . The reason we do this is that it introduces another arbitrary parameter into our model, which confuses the comparison of the different results. Of course, this parameter must be retained in any realistic calculation of the transition temperature.

Now the question is whether a different curve is obtained in the present model, which has two features different from this smooth density of states: the bandwidth is bounded, and the density of states is singular.

In the first calculations we assigned λ an arbitrary and fixed value, and found T_c as a function of the chemical potential -1 < u < 0. For $\lambda = 1.25$, t = 1.0 eV, $\omega_0 = 0.05$ eV the results are shown in Fig. 2. $T_c = 83$ K except for a small upturn near the critical point and a downturn near the lower band edge. This curve is one of our main results.

The value of 83 K is also what one would also get assuming that g = 1. So the critical point in the density of states has no influence on T_c once one is 10% of the bandwidth away from the singular point. We found this was always the case, regardless of the value of λ . In high-temperature superconductors, the occupation of conduction electrons is always 10% away from the Van Hove singularity to avoid antiferromagnetism. Our conclusion is that the critical point has no influence on the transition temperature, since actual superconductors are away from the singularity sufficiently that it has no influence on the answer. Of course, the Van Hove singularity could influence the value of λ .

III. ANGULAR DEPENDENCE

Our interest is to explore the consequences of having the energy gap depend upon an angle. For a square lattice, the Fermi-surface harmonics at the zone center are $\cos(4l\phi)$, where *l* is an integer. In this section we define some important angular functions and explore their properties. Define the functions

$$h_{4l}(u) = 4\pi t a^2 \int \frac{d^2 k}{(2\pi)^2} \cos(4l\phi) \delta(4tu - E_k) , \qquad (21)$$

$$\tan\phi = \frac{k_y}{k_x} . \tag{22}$$

The prefactor to the integral makes these functions dimensionless. The function $h_0(u)$ equals the function h(u) defined and used in the last section. It is proportional to the density of states. For integers l > 0 the functions describe the angular components in the density of states. They vanish for parabolic bands, but are nonzero for any tight-binding model. Later it will be useful to define the ratios

$$r_{4l}(u) = \frac{h_{4l}(u)}{h_0(u)} .$$
⁽²³⁾

These parameters are small for all values of u. They become the basis for the perturbation solution to the gap equations. Figure 3(a) shows numerical results for the band dispersion in (3). We show $h_0(u)$, $h_4(u)$, and $h_8(u)$. One finds that $h_0 > h_4 > h_8$. Figure 3(b) shows $r_4(u)$ and $r_8(u)$. They get very small away from the Van Hove



FIG. 3. (a) Values of h_0 (top), h_4 (middle), h_8 (lower) as a function of u. h_{4l} decreases rapidly with increasing l; (b) $r_4(u)$ (top) and $r_8(u)$ (lower) as a function of u.

singularity.

In cuprate superconductors the conduction electrons are in planes of copper and oxygen ions. A tight-binding model which connects only the in-plane oxygen orbitals has a band dispersion $E_k = \pm A \sin(k_x a/2) \sin(k_y a/2)$. This expression makes contours of constant energy revolve around the corners of the Brillouin zone. It makes sense to redefine the corner of the zone as the center, which effectively changes the band dispersion to

$$E_{\rm k} = \pm A \cos(k_x a/2) \cos(k_y a/2)$$
, (24)

where A = 4t is the width of the occupied band at half filling. We calculated $h_{4l}(u)$ for this case of band dispersion. We found that they were numerically identical to the same functions for band dispersion (3) except that now $h_4(u)$ is negative.

It is interesting to examine (21) in polar coordinates. Define $\theta = ka$ and then we have

$$h_{4l}(u) = \frac{1}{4\pi} \int_{0}^{2\pi} d\phi \cos(4l\phi) \int \theta d\theta \delta(u - E_k/4t) , \quad (25)$$
$$= -\frac{1}{4\pi} \int_{0}^{2\pi} \cos(4l\phi) \left[\frac{\theta d\theta}{2} \right] \quad (26)$$

$$=\frac{1}{4\pi}\int_0^{2\pi}\cos(4l\phi)\left[\frac{\partial u}{\partial u}\right].$$
 (26)

The quantity $(\theta d\theta/du)$ is a function of angle. Since it must be expandable in Fermi-surface harmonics, the above integral defines it as

$$\left|\frac{\partial d\theta}{\partial u}\right| = 2h_0(u) \left[1 + 2\sum_l r_{4l}(u)\cos(4l\phi)\right].$$
(27)

This expression will be needed in solving the Eliashberg equations. It seems to be a new result.

We can also show near the van Hove singularity that as $u \to 0$ then $h_{4l} \to a_{4l} - (2/\pi) \ln |u|$, where $a_0 = 0.883$, $a_4 = -1.180$, $a_8 = -1.951$. Obviously $r_{4l} \to 1$ as $|u| \to 0$. However, this limit is approached very slowly.

The electron-phonon matrix element $M(\mathbf{k}, \mathbf{k}')$ provides the angular dependence for the electron self-energy and the energy gap. We assume that the wave vectors $(\mathbf{k}, \mathbf{k}')$ are on the Fermi line. Then the matrix element can only depend upon the angles (ϕ, ϕ') which these wave vectors make with, say, the x axis. In this case the appropriate form for the interaction is

$$|M(\phi, \phi')|^2 = \sum_{l} m_{4l} \cos(4l\phi) \cos(4l\phi') .$$
 (28)

This form was first derived by Aoi and Swihart.³ Here we give a short explanation. We started by thinking that the most important angular dependence was given by $q = |\mathbf{k} - \mathbf{k}'|$ which depends upon $\cos(\phi - \phi')$. The star of a wave vector are all directions which, by symmetry, have equivalent energy and other properties. The star for the square lattice has eight points except at special angles $(\phi=0, \pi/4)$ where there are four. In doing integrals, one can just evaluate over one-eighth of the Brillouin zone, and then sum over the star. It is easy to show that summing ϕ' over the eight values in its star gives the identity

$$\sum_{\text{star}} \cos[n(\phi - \phi')] = 8\cos(n\phi)\cos(n\phi')$$
(29)

if n = 4l and equals zero otherwise. Even expressions such as $\cos^n(\phi - \phi')$ reduce to the form in (28).

It is also convenient to define a coupling constant for each order of the harmonic expansion. In accord with (8) we define

$$\lambda_{4l} = \frac{2m_{4l}h_0(u)}{c\omega_0 4\pi t a^2} .$$
(30)

As an example of angular behavior, consider the selfenergy of the electron. Starting from (7) we can now write it as

 $\Sigma_n(u,\phi) = 4t \sum_l r_{4l}(u)\sigma_{n,4l}\cos(4l\phi) ,$ (31)

$$\sigma_{n,4l} = \frac{\lambda_{4l} v_0}{2} \int_{-1}^{1} dv \, g_{4l}(v) \left[\frac{N_0 + 1 - n_F(v)}{id(n + \frac{1}{2}) + u - v - v_0} + \frac{N_0 + n_F(v)}{id(n + \frac{1}{2}) + u - v + v_0} \right], \tag{32}$$

$$g_{4l}(v) = \frac{h_{4l}(v)}{h_{4l}(u)} .$$
(33)

We evaluated the integral in $\sigma_{n,4l}$ for l=0,1. In both cases the real part is large and slowly varying, while the imaginary part is smaller and increases from zero at zero imaginary energy. For σ_{n0} we renormalize the chemical potential by the amount at zero imaginary energy. The remaining real part is small and unimportant. However, a similar renormalization of the real part of σ_{n4} does not occur, so that the real part of this expression remains the most important. Furthermore, the imaginary part is not just scaled by $r_4(u)$ over the value for l=0, since the energy variations of the integrand are always important. We did not use $\sigma_{n,4}$ in our solutions to the gap equations.

The energy gap is expanded in Fermi-surface harmonics

$$W(\mathbf{p}, ip_n) = \sum_l W_{n,l} \cos(4l\phi) .$$
(34)

Then the equation for the energy gap, in the approximation of neglecting Coulomb repulsion, is

$$W_{nl} = \lambda_{4l} \sum_{ml'} \frac{W_{ml'} \Lambda_{l,l'}(m)}{1 + b^2 (n-m)^2} , \qquad (35)$$

$$\Lambda_{l,l'}(m) = \frac{d}{2h_0} \int \frac{d^2\theta}{(2\pi)^2} \frac{\cos(4l\phi)\cos(4l'\phi)}{|id(m+\frac{1}{2})+u-E_k/4t-\sigma_m(\phi)|^2}$$
(36)

$$=\frac{1}{|2m+1|}\int_{0}^{2\pi}\frac{d\phi}{2\pi}\cos(4l\phi)\cos(4l'\phi)I_{m}(\phi,u),$$
(37)

$$d_{1}(\phi, u) = d \int \frac{dv}{dv} \frac{1 + 2r_{4}(v)\cos(4\phi) + \cdots}{2}$$
(38)

$$I_{m}(\phi, u) = d \int \frac{dv}{2\pi} \frac{1 + 2 \cdot \frac{1}{4} (v) \cos((\psi) + (1 + \frac{1}{2}) - \mathrm{Im}\sigma_{m})^{2}}{(v - u + \mathrm{Re}\sigma_{m})^{2} + [d(m + \frac{1}{2}) - \mathrm{Im}\sigma_{m}]^{2}}$$
(38)

$$\approx \frac{1}{|2m+1|Z_{m}(\phi)|} [1 + 2r_{4}(u)\cos(4\phi) + \cdots],$$

$$Z_{m}(\phi) = 1 - \operatorname{Im}\sigma_{m}(\phi)/d|m + \frac{1}{2}|.$$
(39)
(40)

$$Z_m(\phi) = 1 - \mathrm{Im}\sigma_m(\phi)/d |m + \frac{1}{2}|$$
.

We used the theorem in (27) to provide the numerator in (38). We ignore the real part of the electron self-energy, which we find to be small. In general, it is useful to write

$$\Lambda_{l,l'}(m) = \frac{\gamma_{l,l'}(m)}{|2m+1|S_m(0)|} .$$
(41)

The important values of $\gamma_{ll'}$ are $\gamma_{00}=1$, $\gamma_{11}=\frac{1}{2}$, and $\gamma_{01} = \gamma_{10} = \xi$. The parameter ξ is proportional to r_4 and is therefore rather small. It also depends slightly upon m. However, this dependence is small, so we ignored it and instead considered it independent of m. This approximation makes the Eliashberg equations easy to solve.

We consider the contribution of the l=0 and 1 levels. Then the gap equations can be written in a matrix form:

$$\mathcal{W}_n = \sum_m v_{n,m} \mathcal{M} \mathcal{W}_m \quad , \tag{42}$$

$$\mathcal{W}_n = \begin{bmatrix} w_{n0} \\ w_{n4} \end{bmatrix} , \tag{43}$$

$$\mathcal{M} = \begin{vmatrix} \lambda_0 & \lambda_0 \xi \\ \lambda_4 \xi & \frac{1}{2} \lambda_4 \end{vmatrix} , \qquad (44)$$

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$$v_{n,m} = \frac{1}{|2m+1|S_m(0)[1+b^2(n-m)^2]}$$
 (45)

The matrix \mathcal{M} has eigenvalues

$$\lambda_{\pm} = \frac{1}{2} [\lambda_0 + \lambda_4/2 \pm \sqrt{(\lambda_0 - \lambda_4/2)^2 + 4\lambda_0 \lambda_4 \xi^2}] .$$
 (46)

The advantage of making ξ independent of m is that the matrix \mathcal{M} is independent of this parameter. Then it is easy to construct matrices $\mathcal{S}, \mathcal{S}_R$ which have the property

$$\mathscr{SS}_{R} = \mathscr{J} , \qquad (47)$$

$$\mathscr{S}_{R}\mathscr{M}\mathscr{S} = \begin{bmatrix} \lambda_{+} & 0\\ 0 & \lambda_{-} \end{bmatrix}, \qquad (48)$$

in which case the gap equations can be written as

$$\mathcal{U}_n = \sum_m v_{n,m} \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} \mathcal{U}_m , \qquad (49)$$

$$\mathcal{U}_n = \mathscr{S}_R \, \mathcal{W}_n \ . \tag{50}$$

Instead of having a matrix of twice the dimension, as in (42), we have two different matrix problems with different values of λ . Obviously λ_+ will give the highest value of T_c . Note that in solving this equation, one still uses λ_0 in evaluating Z_m , so that one has one value of coupling constant in the numerator and a different one in the denominator.

Figure 4 shows numerical results obtained by solving this set of equations. We set $\lambda_0=1$, t=1 eV, $\omega_0=0.05$ eV, and varied λ_4 for $\xi=0.1$ (dashed lines) and 0.2 (solid lines). The two curves in each case are for λ_{\pm} . There is a classic level crossing. If $\xi=0$ then one would have two curves: a $T_c(\lambda_0)$ would be constant since this variable is unchanged, while $T_c(\lambda_4)$ increases with this parameter as in Fig. 1. The two values of T_c would be equal when $\lambda_4=2\lambda_0$. When we have nonzero values of ξ , the two levels repulse each other as is well known for the crossing of two interacting levels. We conclude that the value of T_c is increased in two-dimensional superconductors whenever we have that $\lambda_4 \sim \lambda_0$. In Eq. (28), the second term m_4

150.0

100.0

50.0

 F_{c}

FIG. 4. T_c vs λ_4 for two values of $\xi = 0.1$ (dashed line) and

 $\xi = 0.2$ (solid line). The value of $\lambda_0 = 1.0$ is fixed.



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FIG. 5. Variation in the superconducting energy gap $\Delta(\phi)$ vs angle ϕ for the data reported in Ref. 31. The squares are data points of their sample no. 2. The circles are the present theory, Eq. (1), using $\Delta_0 = 15$ meV and $\Delta_4 = 5$ meV.

has to be similar in size to the first term m_0 . If this condition is met, then the angular variations in the s-wave gap can increase the value of the superconducting transition temperature T_c .

Photoemission has been used to measure the energy gap $\Delta \phi$ around the Fermi line in the cuprate plane.³¹⁻ The original report³² showed that there was little angular dependence and concluded that $\Delta(\phi)$ was a constant, which implied s-wave symmetry. Recent reports³¹ have found angular variation, and even suggested d-wave symmetry. We wish to note that the recent variation can also be fit well by the present theory using s-wave symmetry. Reference 31 reported three sets of data which were not consistent, and each had much scatter. We arbitrarily picked one for illustration, their sample no. 2. Figure 5 shows a graph of the energy gap $\Delta(\phi)$ vs $0 < \phi < \pi/4$. The squares are data points from Ref. 31 while the circles are just $\Delta(\phi) = \Delta_0 + \Delta_4 \cos(4\phi)$ with $\Delta_0 = 15$ meV and $\Delta_4 = 5$ meV. Different values of Δ_4 are obtained from the other samples reported in Ref. 31. We conclude that these data are fit quite well by our theory, and for reasonable values of the parameters.

IV. DISCUSSION

We have solved the Eliashberg equations in two dimensions for the superconducting transition temperature T_c . Of interest are two questions: (1) Does the Van Hove singularity affect the value of T_c ? We find that T_c is increased when the chemical potential is within 10% of the singular energy. However, in high-temperature superconductors, the chemical potential is not that close to the singular energy, so that T_c is not influenced by the Van Hove singularity. (2) Do the angular variations of the energy gap, for s-wave symmetry, increase the value of T_c ? We find that the angular variations introduce additional coupling constants λ_{4l} for each order of angular dependence. Whenever any of these parameters for l > 0 are similar in size to the isotropic value λ_0 then indeed T_c will increase. The increase can be as large as 50%.

So far we have not discussed the variation in the coupling constants λ_{4l} with the van Hove singularity. That is a complex question. Certainly the values of λ have a

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factor of the density of states in the numerator, which suggests they increase as the chemical potential nears the singular energy. However, the electron-phonon matrix element may have additional factors of the density of states. If this matrix element is from the screened Coulomb interaction between electrons and ions, then the screening function contains the density of states. This latter dependence makes λ smaller. Thus, some effects make λ larger, and some make it smaller, as one increases the density of states. The final answer depends upon the precise form for the electron-phonon matrix element. We have also noted that our theory explains the angular variation in the gap reported in recent photoemission experiments.

ACKNOWLEDGMENTS

We wish to acknowledge research support from the National Science Foundation DMR-90-15771, from the University of Tennessee, and from the U.S. Department of Energy through Contract No. DE-AC05-84OR21400 administered by Martin Marietta Energy Systems.

- ¹G. M. Eliashberg, Zh. Eksp. Teor. Fiz. **38**, 966 (1960) [Sov. Phys. JETP **11**, 696 (1960)].
- ²C. S. Owen and D. J. Scalapino, Physica 55, 691 (1971).
- ³K. Aoi and J. C. Swihart, Phys. Rev. B 7, 1240 (1973).
- ⁴P. B. Allen Phys. Rev. B **13**, 1416 (1976).
- ⁵P. B. Allen and B. Mitrović, Solid State Phys. 37, 1 (1982).
- ⁶G. D. Mahan, *Many-Particle Physics*, 2nd ed. (Plenum, New York, 1990).
- ⁷W. E. Pickett, Rev. Mod. Phys. **61**, 433 (1989).
- ⁸J. E. Hirsch and D. J. Scalapino, Phys. Rev. Lett. 56, 2732 (1986).
- ⁹P. A. Lee and N. Read, Phys. Rev. Lett. 58, 2691 (1987).
- ¹⁰D. M. Newns *et al.*, Comments Condens. Mater. Phys. 15, 273 (1992).
- ¹¹C. C. Tsuei *et al.*, Phys. Rev. Lett. **65**, 2724 (1990); **69**, 2134 (1992).
- ¹²P. Horsch and H. Rietschel, Z. Phys. B 27, 153 (1977).
- ¹³B. Mitrović and W. E. Pickett, Phys. Rev. B 35, 3415 (1987).
- ¹⁴E. Schachinger, M. G. Greeson, and J. P. Carbotte, Phys. Rev. B 42, 406 (1990).
- ¹⁵H. Krakauer, W. E. Pickett, and R. E. Cohen, Phys. Rev. B 47, 1002 (1993); Phys. Rev. Lett. 64, 2575 (1990).

- ¹⁶J. H. Nickel, D. E. Morris, and J. W. Ager, Phys. Rev. Lett. 70, 81 (1993).
- ¹⁷G. D. Mahan and J. O. Sofo, Phys. Rev. B 47, 8050 (1993).
- ¹⁸R. J. Radtke et al. (unpublished).
- ¹⁹J. Ruvalds and A. Virosztek, Phys. Rev. B 43, 5498 (1991).
- ²⁰C. M. Varma et al., Phys. Rev. Lett. 63, 1996 (1989).
- ²¹S. M. Cui and C. H. Tsai, Phys. Rev. B 44, 12 500 (1991).
- ²²H. Kaga and T. Saikawa, Physica C 169, 485 (1989).
- ²³R. R. Sharma and H. Lee, J. Appl. Phys. 66, 3723 (1989).
- ²⁴R. W. Wood, M. Mostoller, and J. F. Cooke, Physica C 165, 97 (1990).
- ²⁵D. Markowitz and L. P. Kadanoff, Phys. Rev. 131, 563 (1963).
- ²⁶A. J. Bennett, Phys. Rev. 140, A1902 (1965).
- ²⁷P. B. Allen, Phys. Rev. B 13, 1416 (1976).
- ²⁸G. D. Mahan, Phys. Rev. B 40, 11 317 (1989).
- ²⁹J. A. Martindale et al., Phys. Rev. B 47, 9155 (1993).
- ³⁰D. Thelen et al., Phys. Rev. B 47, 9151 (1993).
- ³¹Z.-X. Shen et al., Phys. Rev. Lett. 70, 1553 (1993).
- ³²C. G. Olson et al., Science 245, 731 (1989).
- ³³D. M. King et al., Phys. Rev. Lett. 70, 3159 (1993).
- ³⁴R. O. Anderson *et al.*, Phys. Rev. Lett. **70**, 3163 (1993).