Superconducting transition temperatures from anisotropic interactions

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The anisotropic electron-phonon interaction is used to calculate the transition temperature T_c of a superconductor. We derive constraints on the maximum value of the anisotropic interaction, and use these extremal values to calculate the maximum increase in T_c from the anisotropy. Calculations are done for electrons on a two-dimensional square lattice using an Einstein model for phonons.

Recent research in high-temperature superconductors has focused on whether the energy gap has d-wave or anisotropic s-wave symmetry.[1-11] Anisotropic s-wave gaps are caused by an anisotropic interaction between electrons on the Fermi surface of the conductor.[12-14] Recently we derived a theory of the anisotropic s-wave interaction for two-dimensional electrons on a square lattice.[12] Here we wish to show how the anisotropic interaction increases the transition temperature of the superconductor. Calculations are done for the electron-phonon interaction with an Einstein model for the phonons.

Our objective is to determine the maximum amount that the anisotropic interaction can increase T_c over an isotropic interaction. Earlier we showed that the interaction can be given in terms of anisotropic coupling constants λ_{4l}. Here we establish bounds on the values of these coupling constants for $l>0$, which then determines bounds on the increase in T_c. In general, we find that the importance of the anisotropic interaction increases as the chemical potential approaches the Van Hove singularity which is always present in two dimensions.

These calculations are an extension of our earlier work in Ref. 12. The present calculations were inspired by the recent paper by Zhao and Callaway[13] who calculate the transition temperature of $YBa_2Cu_3O_7$ using realistic band structure parameters. They used the anisotropic electron-phonon interaction. They find $T_c=63$ K with an isotropic interaction, while including anisotropy increased the value to $T_c=90$ K. Their result verified our earlier ideas[12] that anisotropy increased T_c. However, their increase in T_c is much larger than the values we found. That raises the question of finding the maximum increase in T_c caused by anisotropy. That is the motivation of the present calculation. Our results do not find as large an increase as they reported. However, we are doing a calculation for a single conduction band, and they emphasize that several bands contribute to their final result.

I. ANISOTROPIC INTERACTION

The interaction between electrons in a lattice must conform to the group symmetry of the crystal. Fermi surface harmonics are the set of basis functions which conform to the crystal symmetry.[15-17] Earlier[12] we showed that a simple set of Fermi-surface harmonics for the square lattice are $\cos(4l\phi)$, where l is an integer and $\phi=\arctan(k_y/k_x)$ is the angle which determines the position of the electron on the Fermi surface of energy μ. This definition is useful when $\mu<0$ and the band is less than half filled. Whenever $\mu>0$ we invoke electron-hole symmetry and relabel the band corner as the band center. In two dimensions, the angle ϕ is the only variable needed to describe the position of electrons on the Fermi surface.

The square of the matrix element for the interaction between two electrons on the Fermi surface can be expanded[12,15]

$$|M(\phi,\phi')|^2=\sum_l m_{4l}\cos(4l\phi)\cos(4l\phi') \tag{1}$$

$$=m_0[1+s_4\cos(4\phi)\cos(4\phi')+s_8\cos(8\phi)\cos(8\phi')+\cdots]\,. \tag{2}$$

The usual parameter which denotes the strength of the interaction between electrons and an oscillator of frequency ω_0, such as a phonon or plasmon, is called λ. In the present case there is a value of λ_{4l} for each Fermi-surface harmonic. Below λ_{4l} is defined in terms of the dimensionless density of states $h_0(u)=2K(1-u^2)/\pi$, where K is an elliptic integral and $u=\mu/W$, and $W=4t$ is the bandwidth for a nearest-neighbor hopping model. The Van Hove singularity is at $u=0$. If the lattice has a constant d and the planes are separated by a distance c then the definition of the coupling constant is

$$\lambda_{4l}=\frac{2m_{4l}h_0(u)}{c\omega_0\pi d^2W}\,, \tag{3}$$

$$s_{4l}=\frac{\lambda_{4l}}{\lambda_0}=\frac{m_{4l}}{m_0}\,. \tag{4}$$

We will treat the parameters λ_4 and λ_8 as adjustable within physical limits. Given their full range of possible values, what kind of increase is achieved for the transition temperature? We find that even allowing any value, only a small increase in T_c is achieved.

Another set of parameters required for the expansion

in Fermi-surface harmonics are those related to the density of states. The dimensionless density of states for $\cos(4l\phi)$ is denoted as $h_{4l}(u)$.

$$h_{4l}(u)=4\pi t d^2\int\frac{d^2k}{(2\pi)^2}\cos(4l\phi)\delta(4tu-E_k)\ , \tag{5}$$

$$E_k=-2t[\cos(k_x d)+\cos(k_y d)]\ . \tag{6}$$

The angle ϕ is chosen as $\tan(\phi)=k_y/k_x$ if $u<0$ and according to $\tan(\phi)=(\pi-k_y d)/(\pi-k_x d)$ if $u>0$. This latter choice is due to electron-hole symmetry and makes $h_{4l}(u)$ a symmetric function of u.

Earlier[12] we derived the relation between the wave vector k and the dimensionless energy $u=E_k/W$

$$\frac{kdk}{du}=\frac{2}{d^2}G(u,\phi)\ , \tag{7}$$

$$G(u,\phi)=h_0(u)+2h_4(u)\cos(4\phi)+2h_8(u)\cos(8\phi)+\cdots\ . \tag{8}$$

The function h_4 and h_8 play a key role in the calculation of the gap anisotropy. Values for these functions were given earlier. Generally we find that $h_0<h_4<h_8$. The functions rapidly decrease in value with increasing value of l.

II. MAXIMUM λ_{4l}

There are no bounds that we know on λ_0. Our approach is to assume a value for λ_0 and then ask what constraints are on the anisotropic couplings ($l>0$). First consider that we only include the first two parameters λ_0 and λ_4. The value of λ_4 is constrained by the requirement that the square of the matrix element in (2) be positive, which gives $|\lambda_4|<\lambda_0$. We find that T_c increases with λ_4, so the bound is obtained using its largest value $\lambda_4=\lambda_0$.

Next we add two anisotropic coupling constants λ_4 and λ_8. Again the maximum T_c occurs when λ_4 and λ_8 are as large as possible. Their values are constrained by the requirement that the square of the matrix element in (2) is positive. Neither λ_4 nor λ_8 can exceed λ_0, and both cannot equal it simultaneously. There is a critical value $s_{\rm crit}=(1+1/\sqrt{2})/2=0.8536$. Recalling that $s_l=\lambda_l/\lambda_0$, for $s_8<s_{\rm crit}$ then λ_4 can have its maximum value of λ_0. However, for $s_{\rm crit}<s_8<1$ then $\lambda_4<\sqrt{8\lambda_8(\lambda_0-\lambda_8)}$. We have searched through the parameter space and found that the largest T_c occurs when $\lambda_4=\lambda_0$ and $\lambda_8=\lambda_0 s_{\rm crit}$. These values are used to calculate the effects of the anisotropy.

Our calculations show a significant increase in T_c when including λ_4 but a negligible increase when including λ_8. We assume that the contribution of λ_{12} and higher coefficients is negligible.

III. GAP EQUATION

Earlier we derived an expression for the energy gap for the square lattice. First define the gap function $W(\mathbf{k},ik_n)$ of imaginary energy ik_n as an expansion in Fermi-surface harmonics,

$$W(\mathbf{k},ik_n)=\sum_l W_{nl}\cos(4l\phi)\ . \tag{9}$$

Ignoring Coulomb repulsion, the gap equation for electrons interacting with an oscillator described by an Einstein model has a gap equation[18–20]

$$W_{nl}=\sum_{mk}\frac{W_{mk}\gamma_{lk}(m)}{[1+b^2(n-m)^2]}\ , \tag{10}$$

$$b=\frac{2\pi k_B T_c}{\omega_0}\ , \tag{11}$$

$$\gamma_{lk}(m)=\frac{a\lambda_{4l}}{2\pi h_0(u)}\times\int_{-1}^{1}dv\int_0^{\pi}\frac{d\phi}{\pi}\frac{\cos(4l\phi)\cos(4k\phi)G(u,\phi)}{|ia_m+u-v-\sigma(m,\phi)|^2}\ , \tag{12}$$

$$a=\frac{2\pi k_B T_c}{W}\ , \tag{13}$$

$$a_m=a(m+1/2)\ , \tag{14}$$

$$\sigma(m,\phi)=\frac{\Sigma(m,\phi)}{W}\ , \tag{15}$$

$$=\sum_l\lambda_{4l}\xi_{4l}\cos(4l\phi)\ , \tag{16}$$

$$\xi_{4l}=\frac{\omega_0}{2Wh_0(u)}\int_{-1}^{1}dv h_{4l}(v)\left[\frac{N_0+1-n(v)}{ia_m+u-v-\omega_0/W}+\frac{N_0+n(v)}{ia_m+u-v+\omega_0/W}\right]\ , \tag{17}$$

$$n(v)=1/\{\exp[(v-u)W/k_B T_c]+1\}\ , \tag{18}$$

$$N_0=1/[\exp(\omega_0/k_B T_c)-1]\ . \tag{19}$$

These equations give our theory for the gap equations for an anisotropic s-wave gap. Note that we are doing a strong-coupling calculation which includes the electron self-energy $\Sigma(m,\phi)$ in the electron Green's function.

The integrals over dv were evaluated numerically. The angular integral over $d\phi$ was done analytically. We tried several exact methods which gave poor results due to the small values of ξ_4 and ξ_8. The angular terms in the denominator of (12) have very small coefficients. Finally, we did an approximate evaluation by expanding these small terms into the numerator of the integrand and kept enough terms in the expansion to get convergence.

IV. NUMERICAL RESULTS

We evaluated the above equations for $\lambda_0=1$. This value is arbitrary but does give the same T_c as found by Zhao and Callaway[13] for an isotropic interaction. We fix this value even as we vary in the chemical potential. In a realistic calculation the coupling will change with chemical potential. Changes in the density of states will change the coupling, and also the screening of the coupling. This

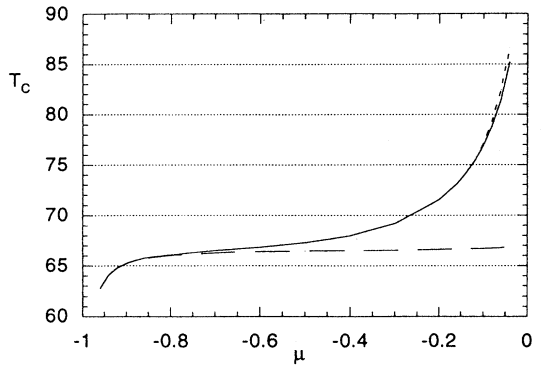

FIG. 1. T_c (in K) as a function of the reduced chemical potential $u=\mu/W$ for three sets of coupling parameters: (i) lower curve has $\lambda_0=1$, $\lambda_4=\lambda_8=0$, (ii) middle curve (solid) has $\lambda_0=\lambda_4=1$, $\lambda_8=0$, and (iii) top curve has $\lambda_0=\lambda_4=1$, $\lambda_8=0.8548$. The bottom of the band is at $u=-1$ and the midpoint of the band is at the Van Hove singularity at $u=0$. The anisotropy parameters λ_4,λ_8 have increasing effect near the Van Hove singularity where the energy band is more anisotropic.

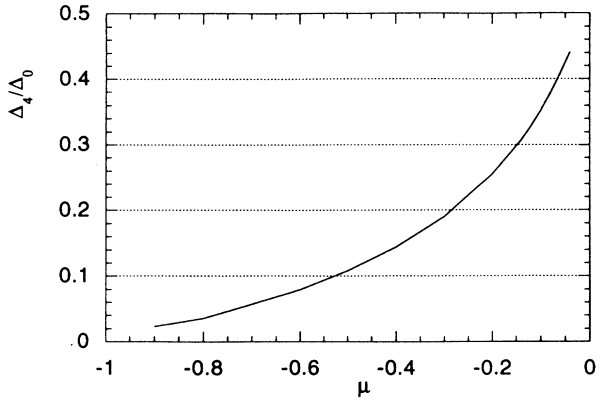

FIG. 2. Ratio of $\Delta_4(\omega=0)$ to $\Delta_0(\omega=0)$ at T_c when $\lambda_0=\lambda_4=1.25$ and $\lambda_8=0$. Both Δ_0 and Δ_4 are infinitesimal at the transition temperature. Their ratio shows the degree of gap anisotropy. The result depends upon how close the chemical potential is to the van Hove singularity at $\mu=0$.

effect is rather complex, and beyond the scope of the present calculation. The phonon energy is $\omega_0=50$ meV. This value is close to the midpoint of the phonon spectrum of the cuprates, and close to the peak in α^2F at 60 meV found by Zhao and Callaway. This peak dominates α^2F. The bandwidth was taken to be $t=1.0$ eV or $W=4.0$ eV.

The results are shown in Fig. 1. The lower curve shows the value of T_c as a function of $-1<u<0$ for the isotropic interaction ($\lambda_4=\lambda_8=0$). We find that $T_c=66.5$ K over much of the occupied band. The value of T_c falls at the left as the number of electrons in the band starts to vanish. The value of T_c seems unchanged for the isotropic interaction as the chemical potential approaches the Van Hove singularity which is at $u=0$.

The solid line in Fig. 1 is the result obtained using $\lambda_0=\lambda_4=1$ and $\lambda_8=0$. The value of T_c rises near the Van Hove singularity at $u=0$ but joins the curve with $\lambda_4=0$ at the bottom of the band near $u=-1$. The difference between the curves with and without λ_4 mimics the behavior of $h_4(u)$. This function is zero at $u=-1$ and rises at the Van Hove singularity. The function $h_4(u)$ provides the coupling between λ_4 and λ_0. As we raise u, this coupling (h_4) increases, and the contribution of λ_4 has a large effect. At $u=-0.2$ the increase in T_c is about 10% and at $u=-0.1$ the increase is about 20%.

At values of u approaching zero, Fig. 1 shows a dashed line slightly above the solid line. The dashed line includes the influence of λ_8. This curve was calculated using the values of $\lambda_0=\lambda_4=1$ and $\lambda_8=0.8536$. The coupling parameter λ_8 enters through the function $h_8(u)$ or else h_4^2 and both of these are very small except very near to the Van Hove singularity. Even at $u=-0.04$ the increase in T_c due to λ_8 is only about one degree.

Since we solve the gap equation at T_c the energy gap is zero. The matrix in (10) has eigenvectors, and those for eigenvalue unity are the infinitesimal energy gaps $\Delta_{4l}(n+1/2)$. We extrapolate those to zero energy and Fig. 2 shows a plot of Δ_4/Δ_0 at zero frequency. This is graphed for $\lambda_0=\lambda_4=1.25$. It shows the admixture of gap anisotropy as one approaches the Van Hove singularity. The admixture is about 25% when $\mu=-0.2$. For the same parameters the change in T_c is only about 10%. This is the usual result in quantum mechanics, where perturbations change wave functions more than eigenvalues.

At $u=0$ the electron gas on the square lattice is antiferromagnetic and not superconducting. The cuprates must be doped to change the chemical potential away from the Van Hove singularity before superconductivity is achieved. This change in the chemical potential must be on the order of at least 10% of the bandwidth. At $u=-0.10$ the influence of λ_8 is negligible compared to that of λ_4. We conclude that only the first anisotropy parameter λ_4 is important in actual materials. Then the maximum increase in T_c is less than 20%. This is a much smaller increase than the 40% found by Zhao and Callaway. However, their calculation showed several electron bands participated in the conduction process. The multiband aspect of their calculation could explain the differences in our result.

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