Static Coulomb model for high-temperature superconductivity

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Superconductivity in copper oxide planes is calculated using the static Coulomb model. This model is based upon the attractive nature of the Fourier transform of the Coulomb interaction for wave vectors near $a\mathbf{Q}=\pi(\pm1,\pm1)$. Values of λ and $\Delta(\mathbf{k})$ are calculated at $T=0$ and also at T_c where the gap equation becomes a linear matrix equation. For some regions of parameter space values of λ are near unity. The gap $\Delta(\mathbf{k})$ is anisotropic.

Many theoretical models have been introduced to explain high-temperature superconductivity. Two broad classifications are models based upon spin fluctuations[1-4] and upon charge fluctuations.[5-11] The present model is neither, but relies only upon the properties of the statically screened Coulomb interaction.[12,13] The standard tight-binding model for the σ bonding in the copper oxide plane predicts that the Coulomb potential has regions of Fourier space where it is attractive. Under certain circumstances, this attraction predicts superconductivity.

Our version of the static Coulomb model has two parameters. One is the chemical potential $\mu=A\eta$, where $A\sim2$ eV is the bandwidth parameter in the tight-binding theory, which is deduced from band-structure calculations.[14,15] The parameter $\eta\sim1$ is dimensionless and relates to the band filling. A half-filled band has $\eta=1$, and the tight-binding bands from σ bonds allows a range of values of $0<\eta<\sqrt{2}$. The second parameter is the coupling constant $g=e^2/(\epsilon_0 Aa\pi^2)$ where $a=3.86$ Å is the lattice constant. Here we provide a phase diagram which shows the superconducting regions as a function of η and g. The presence of superconductivity is found by solving for the coupling constant λ which enters the energy gap $\Delta\sim2\xi_0\exp(-1/\lambda)$. Usually λ denotes the attractive strength from some oscillator, while U (or μ) denotes the repulsive Coulomb part. Here the notation is different, since we define λ as the total Coulomb integral, which contains both repulsive and attractive contributions.

I. TIGHT-BINDING BANDS

We use the standard three-band model for the σ bonds. The tight-binding model has three orbitals per unit cell: a $d_{x^2-y^2}$ on the copper, and p_x and p_y on the two oxygens. The Hamiltonian is

$$H=\sum_j\left[E_d d_j^\dagger d_j+E_p(c_{jx}^\dagger c_{jx}+c_{jy}^\dagger c_{jy})+(iA/2)d_j^\dagger\sum_\delta[\mathrm{sgn}(\delta_x)c_{j'x}+\mathrm{sgn}(\delta_y)c_{j'y}]+\mathrm{H.c.}\right], \tag{1}$$

where j' are the oxygen neighbors of the copper atoms at j. We assume that $E_p=E_d$. The Hamiltonian can be diagonalized in k space. There are three bands, and the conduction band is the highest in energy. Its energy with respect to the Fermi energy $E_F=A\eta$ is $\xi(k)=A[S(k)-\eta]$, where

$$S(\mathbf{k})=[\sin^2(k_x a/2)+\sin^2(k_y a/2)]^{1/2}.$$

The other two bands have lower energy and are completely filled with electrons. The conduction band has a tight-binding wave function given by

$$\Psi_{\mathbf{k}}(\mathbf{r})=[\phi_d(\mathbf{k},\mathbf{r})+B_x(\mathbf{k})\phi_x(\mathbf{k},\mathbf{r})+B_y(\mathbf{k})\phi_y(\mathbf{k},\mathbf{r})]/\sqrt{2},$$
$$B_\mu(\mathbf{k})=\sin(k_\mu a/2)/S(\mathbf{k}). \tag{2}$$

The functions $\phi_\alpha(\mathbf{k},\mathbf{r})$ with $\alpha=(d,x,y)$ are the Bloch functions for the three localized orbitals. The wave functions $\Psi_k(\mathbf{r})$ are used to calculate the Coulomb interaction for scattering two electrons initially in states $\mathbf{k}$ and $\mathbf{k}'$ to the final states $\mathbf{k}+\mathbf{q}$ and $\mathbf{k}'-\mathbf{q}'$:

$$V(\mathbf{k},\mathbf{k}',\mathbf{q})=\frac{e^2}{\epsilon_0}\int\frac{d^2r_1 d^2r_2}{|\mathbf{r}_1-\mathbf{r}_2|}\Psi^*_{\mathbf{k}+\mathbf{q}}(\mathbf{r}_1)\Psi_{\mathbf{k}}(\mathbf{r}_1)\Psi^*_{\mathbf{k}'-\mathbf{q}}(\mathbf{r}_2)\Psi_{\mathbf{k}'}(\mathbf{r}_2),$$
$$V(\mathbf{k},\mathbf{k}',\mathbf{q})=(e^2/4\epsilon_0 a)T(\mathbf{k},\mathbf{k}',\mathbf{q}).$$

In the second line the quantity $e^2/(4\epsilon_0 a)$ is factored out to make T dimensionless. The interaction T goes as $8\pi/qa$ at small values of q. It is periodic in reciprocal space; the interaction is unchanged if a reciprocal-lattice vector is added to either $\mathbf{k}$, $\mathbf{k}'$, or $\mathbf{q}$. An explicit equation for T is

$$T(\mathbf{k},\mathbf{k}',\mathbf{q})=t(0,\mathbf{q})[1+B_x(\mathbf{k})B_x(\mathbf{k}')B_x(\mathbf{k}+\mathbf{q})B_x(\mathbf{k}'+\mathbf{q})+B_y(\mathbf{k})B_y(\mathbf{k}')B_y(\mathbf{k}+\mathbf{q})B_y(\mathbf{k}'+\mathbf{q})]$$
$$+t(\tau_x,\mathbf{q})[B_x(\mathbf{k})B_x(\mathbf{k}+\mathbf{q})+B_x(\mathbf{k}')B_x(\mathbf{k}'+\mathbf{q})]+t(\tau_y,\mathbf{q})[B_y(\mathbf{k})B_y(\mathbf{k}+\mathbf{q})+B_y(\mathbf{k}')B_y(\mathbf{k}'+\mathbf{q})]$$
$$+t(\tau_{xy},\mathbf{q})[B_x(\mathbf{k})B_x(\mathbf{k}+\mathbf{q})B_y(\mathbf{k}')B_y(\mathbf{k}'+\mathbf{q})+B_y(\mathbf{k})B_y(\mathbf{k}+\mathbf{q})B_x(\mathbf{k}')B_x(\mathbf{k}'+\mathbf{q})] ,$$

$$t(\tau,\mathbf{q})=\sum_j \exp[i\mathbf{q}\cdot(\mathbf{R}_j-\tau)]/|R_j-\tau| ,$$

where $\tau_x=a(\frac{1}{2},0)$, $\tau_y=a(0,\frac{1}{2})$, and $\tau_{xy}=a(\frac{1}{2},\frac{1}{2})$.

For superconductivity we actually need $T(\mathbf{k},-\mathbf{k},\mathbf{q})$. This quantity is easy to calculate using Ewald summations for $t(\tau,\mathbf{q})$. For small values of q one finds that $T=8\pi/qa$, as expected. But for values of $\mathbf{q}\sim\mathbf{Q}=\pi(\pm1,\pm1)/a$, then T is negative. The precise value depends upon $\mathbf{k}$. It is the factor $t(0,\mathbf{Q})$ which is negative.

The Fermi surface in two dimensions is a closed loop which we call the Fermi line (FL). For $\eta\sim1$ then $\mathbf{Q}$ is the vector which spans the FL. The Coulomb interaction is attractive for exchange scattering of two electrons across the FL. It is this feature which is the basis for our static Coulomb model of superconductivity. So far, our remarks pertain to the unscreened interaction. The role of screening is always important. Here it plays a crucial role in our model of superconductivity, as is explained later.

II. SCREENING

In the random-phase approximation (RPA) the screened interaction is the solution to the integral equation

$$\bar{V}(\mathbf{k},\mathbf{k}',\mathbf{q})=V(\mathbf{k},\mathbf{k}',\mathbf{q})+\int\frac{d^2p}{(2\pi)^2}V(\mathbf{k},\mathbf{p},\mathbf{q})\bar{V}(\mathbf{p},\mathbf{k}',\mathbf{q})L(\mathbf{p},\mathbf{q}) , \tag{3}$$

$$L(\mathbf{p},\mathbf{q})=2\frac{n_F(\xi_p)-n_F(\xi_{p+q})}{\xi_p-\xi_{p+q}} .$$

The quantity which enters the gap equation is $\bar{V}(\mathbf{k},-\mathbf{k},\mathbf{q})$. The unscreened quantity $V(\mathbf{k},-\mathbf{k},\mathbf{q})$ is negative for wave vectors in the region around $\mathbf{Q}a=\pi(\pm1,\pm1)$.

The dielectric function must be introduced carefully. For inhomogeneous systems the susceptibility $\chi(\mathbf{r},\mathbf{r}')$ is doubly Fourier transformed and inverted to give the dielectric function $\epsilon(\mathbf{q},\mathbf{q}')$. We lack the resources to do this quickly. Instead we tried to construct a simple dielectric function $\epsilon(\mathbf{q})$ which is a periodic in reciprocal space. We attempted to solve (3) by using the approximate expression $\bar{V}=V/\epsilon$ where the dielectric function is

$$\epsilon(\mathbf{q})=1-\int\frac{d^2k}{(2\pi)^2}V(\mathbf{k},-\mathbf{k},\mathbf{q})L(\mathbf{k},\mathbf{q}) ,$$
$$L(\mathbf{k},\mathbf{q})\approx-2\delta(\xi_k) . \tag{4}$$

This choice has the virtue that it does behave as $\epsilon\approx1+c/q$ at small q, and is also periodic in reciprocal space. This dielectric function has another interesting property. It is less than unity for the spanning vectors $a\mathbf{Q}=\pi(\pm1,\pm1)$. The screening makes the interaction across the FL more attractive, while making the small-q interactions less repulsive. Screening increases the tendency for superconductivity:

$$\epsilon(\mathbf{q})=1+\frac{\eta g}{2(2-\eta^2)}\int_0^{\pi/2}\frac{d\alpha}{[1-m\sin^2(\alpha)]^{1/2}}\times\sum_{i=1}^{8}T(\mathbf{k},-\mathbf{k},\mathbf{q}) . \tag{5}$$

where $m=[\eta^2/(2-\eta^2)]^2$ if $\eta<1$. The summation is over the star of the wave vector $\mathbf{k}$, where one point for $\eta<1$ is given by

$$\sin(k_x a)=\eta\sin(\pi/4-\alpha/2) .$$

In (5) we have given the dielectric function for $\eta<1$. For $\eta>1$ change η^2 to $2-\eta^2$ except in the prefactor of η.

For $\eta\sim1$ the integral becomes large because of the large density of states at the Fermi energy. For values of $\mathbf{q}$ near the spanning wave factor $a\mathbf{Q}=\pi(\pm1,\pm1)$ the integral is negative. Since it is both large and negative then $\epsilon(\mathbf{Q})<0$. Figure 1 shows a phase diagram calculated for this model in terms of the two parameters g and η. To the right is a region of high values of g where $\epsilon(\mathbf{Q})<0$. This region is separated by a solid line. Since $\epsilon(\mathbf{q})$ is periodic in wave vector, we assume that the most negative point is at $\mathbf{q}=\mathbf{Q}$. This feature was verified for every case we investigated, but we have no proof that it is always true. A negative values of the dielectric function in-

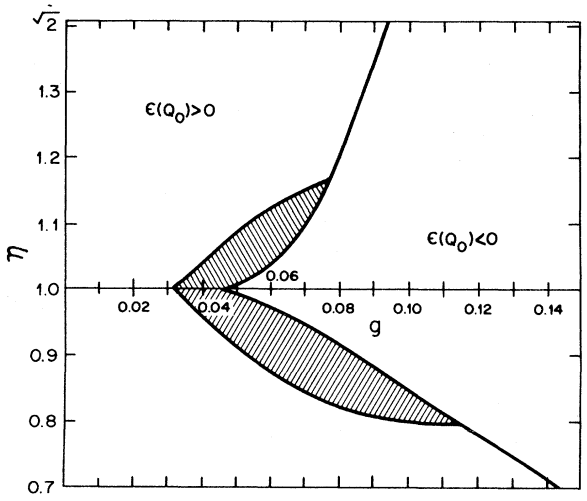

FIG. 1. Phase diagram for the static Coulomb model. The parameter η denotes the chemical potential, while g is the Coulomb coupling coefficient. The line $\eta=1$ is a half-filled band where the two-dimensional density of states is singular. The solid line divides the region on the right where $\epsilon(\mathbf{Q})<0$, where $\mathbf{Q}a=\pi(\pm1,\pm1)$, from the region on the left where $\epsilon(\mathbf{Q})>0$. The right-hand region with $\epsilon(\mathbf{Q})<0$ is unstable and must change to another phase. The shaded region on the left denotes the region of superconductivity as determined by the condition that $\lambda\geq0$. The coupling constant λ is calculated at zero temperature using (8).

dicates an instability. The nature of this instability has not been investigated. To the left of this line is the region where the dielectric function is positive. The region of positive $\epsilon(\mathbf{q})$ has been investigated here. The shaded region is where we find a superconducting phase, as described in Sec. III.

III. SUPERCONDUCTIVITY

The superconductivity energy gap $\Delta(\mathbf{k})$ in weak coupling obeys the equation at zero temperature of[16]

$$\Delta(\mathbf{k})=-\int\frac{d^2k'}{(2\pi)^2}\frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')}\bar{V}(\mathbf{k}',-\mathbf{k}';\mathbf{k}-\mathbf{k}')\ ,$$
$$E(\mathbf{k})=[\xi(\mathbf{k})^2+\Delta(\mathbf{k})^2]^{1/2}\ . \tag{6}$$

The overbar on the potential denotes a screened interaction. In solving the gap equation (6), the wave vector coordinates are changed to a line integral dk_l around the FL and a wave vector $dk_\perp$ perpendicular to the FL, $d^2k'=dk_l dk_\perp$. We assume that the gap function $\Delta(\mathbf{k})$ and Coulomb interaction are slowly varying near the FL. Thus the main contribution to $dk_\perp$ is from the kinetic energy

$$\int dk_\perp\frac{1}{E(\mathbf{k}')}=\frac{4\eta}{A\beta}\ln(2\xi_0/\Delta)\ ,$$
$$\beta(k_l)=\cos(\phi)\sin(k_x a)+\sin(\phi)\sin(k_y a)\ ,$$

where $\xi_0\sim A$ is a cutoff energy, ϕ is the polar angle during the FL integral, and (k_x,k_y) are the wave vectors at the FL of that polar angle. The gap equation (6) can be rewritten as

$$\Delta(k_l)=-\eta g\frac{a}{4}\int dk_l'\Delta(k_l')\ln(2\xi_0/\Delta)T(\mathbf{k}',-\mathbf{k}',\mathbf{k}-\mathbf{k}')/[\beta(k_l)\epsilon(\mathbf{k}-\mathbf{k}')]\ ,$$
$$g=e^2/(\epsilon_0 a A\pi^2)\ . \tag{7}$$

The coupling constant g is one of the two important parameters of the theory. The other is the dimensionless Fermi energy $\eta\sim1$. In order to estimate g, we choose $a=3.68$ Å, $A\approx2$ eV from the bandwidth,[14,15] and $\epsilon_0\leq\epsilon_\infty\approx3$.[17] For $\epsilon_0=3$ we find $g=0.06$, which represents the maximum possible value of the coupling constant.

The preceding line integral has no solution for the case of no screening [$\epsilon(\mathbf{k}-\mathbf{k}')=1$], since the integral is always positive. The weak attractive regions across the FL are insufficient to overcome the strong repulsive regions at small values of $\mathbf{q}=\mathbf{k}-\mathbf{k}'$. Screening is needed to overcome this strong repulsion at small $\mathbf{q}$.

The existence of superconductivity is inferred by calculating the average value of λ around the FL

$$\lambda=-\eta g\frac{a}{4}\int dk_l\int dk_l'\frac{T(\mathbf{k}',-\mathbf{k}',\mathbf{k}-\mathbf{k}')}{\beta(k_l)\epsilon(\mathbf{k}-\mathbf{k}')}\Big/\int dk_l\ , \tag{8}$$

where all integrals are around the Fermi line. The shaded regions in Fig. 1 denote where λ is positive. Note that the calculation has been carried to values of g about twice the expected maximum of 0.06, in order to find the limits of superconductivity for this type of model.

Values of λ are largest, and approach unity, near the line denoting where $\epsilon(\mathbf{Q})=0$, while the other boundary is where $\lambda=0$. The regions of high-temperature superconductivity are near the line where $\epsilon(\mathbf{Q})=0$. Here one has that $\epsilon(q)<1$ for the regions of large q, and the attractive interactions across the FL are increased. The decrease of the small-q repulsion and the increase of the large-q attraction both tend to make the integral in the gap equation (7) more negative, and hence enhance superconductivity. The existence of superconductivity in this model depends in a sensitive way upon the two parameters g and η.

The parameter λ, and the phase diagram for superconductivity, has been calculated a second way. At the transition temperature T_c for superconductivity, the gap equation becomes a linear integral equation

$$\Delta(\mathbf{k}) = -\int \frac{d^2k'}{(2\pi)^2}\Delta(\mathbf{k}')\tanh(\beta_c\xi_{k'}/2)V(\mathbf{k}',-\mathbf{k}',\mathbf{k}-\mathbf{k}')/2\xi_{k'} ,$$

where $\beta_c = 1/k_B T_c$. The integral d^2k' is evaluated as before by separating it into an integral dk_l around the FL plus an integral $d\xi_{k'}$ perpendicular to the FL. The latter integral is defined as $1/\lambda$:

$$\begin{aligned} 1/\lambda &= \int d\xi' \tanh(\beta_c\xi'/2)/\xi' \approx 2\ln(1.134\xi_0\beta_c) , \\ 0 &= \int dk_l' \left[\lambda\delta(k_l - k_l') - \frac{g\eta a T(\mathbf{k}',-\mathbf{k}',\mathbf{k}-\mathbf{k}')}{4\beta(k_l')\epsilon(\mathbf{k}-\mathbf{k}')}\right]\Delta(k_l') . \end{aligned} \tag{9}$$

Equation (9) cast the gap equation into the form of a linear integral equation. The parameter λ is the largest eigenvalue. The integral equation was solved by changing the continuous integral to a summation over a finite number of $\mathbf{k}$ points. It is then a matrix equation which is solved by matrix inversion to obtain the eigenvalues and eigenvectors. Because of the periodicity of $\Delta(\mathbf{k})$ around the FL, the matrices have rather small dimension.

Figure 2 shows the value of λ calculated with this formula compared with the previous results using (8) at zero temperature. The solid line is the result from (9), while the dashed line is the result from (8). Both curves are for $g = 0.060$ and are shown as a function of the filling factor η. The upper limit of this curve terminates where $\epsilon(\mathbf{Q}) < 0$. The two curves are obviously very similar. The two definitions of the gap equation give similar results for other values of g.

The solid line in Fig. 2 ends at $\eta = 0.92$. Below this value we find that the eigenvalue λ is small and complex. The interaction matrix is real but asymmetric, which permits complex eigenvalues. This generally happens when the eigenvalue becomes small. Initially we worried about the behavior of λ in this region. Finally we realized that this region did not show high-temperature superconductivity because of the small values of λ. We adopted an arbitrary cutoff of $\lambda > 0.1$ which avoided the question of complex eigenvalues, which always happened at smaller values. Figure 3 shows a phase diagram for superconductivity obtained by solving Eq. (9). The shaded regions are superconducting, as defined by the two limits that $\epsilon(\mathbf{Q}) > 0$ and $\lambda > 0.10$. This result should be compared with the similar diagram in Fig. 1. The difference in the two diagrams reflects the different behavior at small values of λ. In Fig. 1 the outer boundary was defined where Eq. (8) had $\lambda > 0$, while in Fig. 3 it is where Eq. (9) had $\lambda > 0.10$. The difference in the diagrams is mostly due to the different cutoffs for λ, rather than to the different equations for λ. As shown in Fig. 2, the different calculations of λ differ little except when the eigenvalue is very small.

Equation (9) also provides information regarding the eigenfunctions, which predicts how the gap varies around

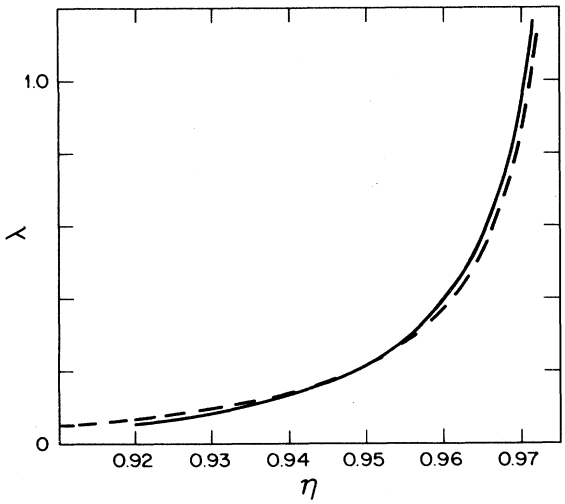

FIG. 2. A graph of λ vs η for $g = 0.060$. The solid line is calculated at T_c as the largest eigenvalue of Eq. (9). The dashed line is calculated at $T = 0$ using (8). The two calculations agree.

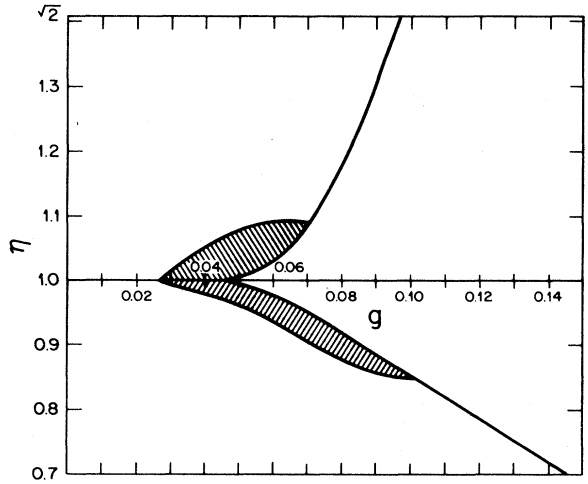

FIG. 3. Phase diagram for the static Coulomb model calculated at T_c. The solid line marks the boundary where $\epsilon(\mathbf{Q}) < 0$ to the right. The superconducting region is shown as shaded. The other boundary is found from the condition that $\lambda > 0.1$ where λ is the largest eigenvalue of (9).

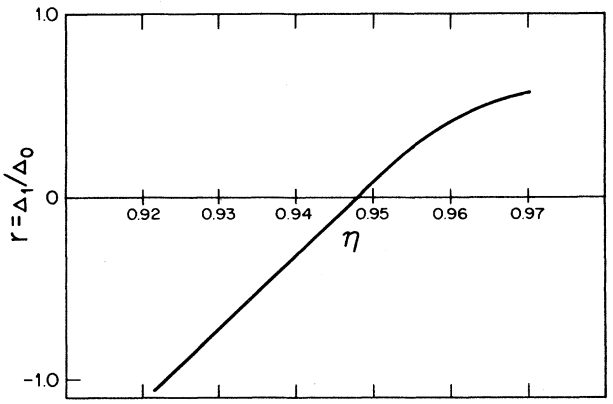

FIG. 4. A graph of the gap anisotropy parameter $r=\Delta_1/\Delta_0$ vs the filling factor η for $g=0.060$.

the FL. Our theory assumes s-wave symmetry, so that the gap has the same values in the $\pm x$ and $\pm y$ directions. However, it can and does vary between these points. For a square lattice the most general form for a Kubic harmonic expansion of the gap is

$$\Delta(\phi)=\sum_n \Delta_n \cos(4n\phi)\approx\Delta_0+\Delta_1\cos(4\phi)$$
$$=\Delta_0[1+r\cos(4\phi)] .$$

The variation in the gap $\Delta(\mathbf{k})$ around the FL has been fitted to a simple $\cos(4\phi)$ law. This fitting provides the parameter r, which is the ratio $r=\Delta_1/\Delta_0$. the magnitude of the gaps Δ_0 and Δ_1 varies with temperature and is zero at T_c. An example of our results for r is shown in Fig. 4 as a function of η for the case that $g=0.060$. Values of r with magnitude greater than 1 signify that the gap can be zero at eight points around the FL. This only happens in our calculations when λ is small. Comparing Fig. 2 for λ with Fig. 4 for r shows that we have $r\sim 0.5$ in the region of high T_c where λ is large. This gap anisotropy should be evident in electron tunneling, as is discussed elsewhere. For other values of g we find an r of similar magnitude, but with either sign. These results for r depend somewhat on the size of the matrix which is inverted. So Fig. 4 should be regarded only as an indicator of the type of anisotropy which may occur in the energy gap.

In summary, we have used the static Coulomb model to calculate a phase diagram for superconductivity in terms of the parameter of the model. We show that values of λ near unity are predicted, which does predict high-temperature superconductivity. We also calculate the anisotropy of the energy gap.

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