# Electron-ion interaction in a nearly ferroelectric metal

Joel I. Gersten

*Department of Physics, City College of New York, New York, New York 10031*

Meir Weger

*Racah Institute of Physics, Hebrew University, Jerusalem, Israel*

We calculate the electron-ion potential for a thin metallic layer (in the $a$-$b$ plane) sandwiched between two semi-infinite dielectrics. The dielectric constant of the dielectrics varies strongly in the $a$-$b$ plane. We show that there is an overscreening effect, and the electron-ion interaction is strongly enhanced, for certain values of the parameters. This suggests the possibility of a greatly enhanced electron-phonon coupling in a nearly ferroelectric metal, such as the high-$T_c$ perovskites.

## I. INTRODUCTION

Recently, materials have been discovered that possess a very high ionic dielectric constant ($\varepsilon_{ion} \approx 20$–$100$), and thus are nearly ferroelectric, yet they possess conduction electrons with a well-defined Fermi surface. Examples are the high-$T_c$ cuprates, such as YBaCuO (YBCO), LaSrCuO, and the other materials of this family; intermediate-$T_c$ materials such as BaKBiO (BKBO); organic metals of the (BEDT-TTF)$_2 X$ family; and Na-doped WO$_3$. The high ionic dielectric constant is usually characteristic of insulators. Thus, having a metal possessing such a large dielectric constant seems to be self-contradictory, since one would expect the conduction electrons to screen out the ionic dielectric constant. In the layered two-dimensional cuprates, this anomalous behavior occurs since the ionic dielectric constant is the component $\varepsilon_{cc}$ in the $c$-direction, while the conduction electron susceptibility $\chi_{el}$ has components in the $a$-$b$ plane, namely, $\chi_{aa}$, $\chi_{bb}$, so that the two can coexist. However, in BKBO, as well as the organic metals, the conduction electrons just do not screen out the ionic dielectric constant.

We calculated the electron-electron scattering in a material with a large dielectric constant a few years ago.[1] The scattering rate is very weak close to the Fermi surface ($|E_k - E_F| < \hbar \omega_{trans}$, where $\omega_{trans}$ is the dispersion frequency of the dielectric constant), and very strong further away for the Fermi surface. Experimentally, such a behavior is observed in the infrared spectra;[2] however, the experimental behavior can also be accounted for in other ways (e.g., a pseudogap that can be due to a variety of causes).

The ionic dielectric constant also affects the conduction electron–ion interaction. In a homogeneous, three-dimensional (3D) system, the Fourier transform of this potential is given by[3]

$$V_{e-ion}(q) = \frac{4\pi Z e^2 / \varepsilon_{ion}(q)}{q^2 + q_D^2 / \varepsilon_{ion}(q)}, \qquad (1)$$

where $q_D^2 = 4\pi e^2 N(0)$ is the Thomas-Fermi screening parameter, and $N(0)$ is the density of states at the Fermi level. Thus, $V_{e-ion}(q)$ is *reduced* by the dielectric, except at $q=0$,

where $\varepsilon_{ion}$ cancels out in the numerator and denominator, and thus $V_{e-ion}(0)$ is unchanged from the unscreened value.

In an inhomogeneous system, the expression for $V_{e-ion}(q)$ is more complex. In a previous publication we considered a crude approximation[3] and suggested that $\varepsilon_{ion} > 1$ may actually *increase* $V_{e-ion}$ over the $\varepsilon_{ion} = 1$ value. We calculated there the value of the superconducting transition temperature $T_c$, and suggested that it is increased significantly by this effect, and can reach a value of about 200 K in cupratelike materials, for a phonon-mediated interaction. Here we consider a specific model of a layered system, and calculate $V_{e-ion}$ for it explicitly.

We consider a thin metallic layer (in the $x$-$y$ plane) surrounded by an insulating ionic dielectric (extending to infinity in the $\pm z$ direction). The bare Coulomb interaction is screened both by the dielectric, and by the electron gas in the metallic layer. The screening by the electron gas is affected by the dielectric and its screening effect is in turn reduced by the dielectric environment. Normally, the direct screening by the dielectric is stronger than the indirect effect of the reduction of the electron screening by it. Consequently, the overall effect of the dielectric is to reduce the strength of the potential, as given by Eq. (1). However, under some exceptional circumstances the indirect effect may be stronger that the direct effect, and then the overall strength of the potential is *increased* by the dielectric.

## II. PRESENCE OF BOTH IONIC AND ELECTRONIC SUSCEPTIBILITIES

The interrelationship of electronic and ionic susceptibilities is treated in the Bardeen-Pines theory. As shown in textbooks,[4] we can write (the polarizations of the ions and electrons add to give the polarizability of the medium)

$$\varepsilon = \varepsilon_{ion}^{dressed} + \varepsilon_{el}^{bare} - 1 = \varepsilon_{el}^{dressed} + \varepsilon_{ion}^{bare} - 1, \qquad (2a)$$

where

$$\varepsilon_{ion}^{dressed} - 1 = (\varepsilon_{ion}^{bare} - 1) / \varepsilon_{el}^{dressed} \qquad (2b)$$

and

$$\varepsilon_{el}^{dressed} - 1 = (\varepsilon_{el}^{bare} - 1)/\varepsilon_{ion}^{dressed}. \tag{2c}$$

Thus, given $\varepsilon_{ion}^{bare}$, $\varepsilon_{el}^{bare}$, we can calculate the dressed quantities and the total dielectric constant $\varepsilon$.

In the Bardeen-Pines theory, $\varepsilon_{el} \ll \varepsilon_{ion}$, therefore we can solve the equations by iteration,

$$(\varepsilon_{ion}^{dressed} - 1)^{(1)} = (\varepsilon_{ion}^{bare} - 1)/\varepsilon_{el}^{bare} \tag{3a}$$

and

$$(\varepsilon_{el}^{dressed} - 1)^{(1)} = (\varepsilon_{el}^{bare} - 1)/(\varepsilon_{ion}^{dressed})^{(1)}$$
$$= (\varepsilon_{el}^{bare} - 1)[\varepsilon_{el}^{bare}/(\varepsilon_{el}^{bare} + \varepsilon_{ion}^{bare} - 1)], \tag{3b}$$

where the superscript (1) indicates the first step of iteration. Since $\varepsilon_{el} \gg \varepsilon_{ion}$, the results of the first iteration step are sufficiently close to the exact result. This is the formula given in Aschcroft and Mermin.[4]

In the opposite limit, namely, $\varepsilon_{el} \gg \varepsilon_{ion}$, we must reverse the order of iteration,

$$(\varepsilon_{el}^{dressed} - 1)^{(1)} = (\varepsilon_{el}^{bare} - 1)/\varepsilon_{ion}^{bare} \tag{4a}$$

and

$$(\varepsilon_{ion}^{dressed} - 1)^{(1)} = (\varepsilon_{ion}^{bare} - 1)/(\varepsilon_{el}^{dressed})^{(1)}$$
$$= (\varepsilon_{ion}^{bare} - 1)[\varepsilon_{ion}^{bare}/(\varepsilon_{ion}^{bare} + \varepsilon_{el}^{bare} - 1)] \tag{4b}$$

We call this the "nearly ferroelectric limit." [5]

In the general case, the solution is

$$\varepsilon_{el}^{dressed} = 1 + \tfrac{1}{2}[\sqrt{(1 + \varepsilon_{ion}^{bare} - \varepsilon_{el}^{bare})^2 + 4(\varepsilon_{el}^{bare} - 1)}$$
$$- (1 + \varepsilon_{ion}^{bare} - \varepsilon_{el}^{bare})] \tag{5a}$$

and

$$\varepsilon_{ion}^{dressed} = 1 + \tfrac{1}{2}[\sqrt{(1 + \varepsilon_{el}^{bare} - \varepsilon_{ion}^{bare})^2 + 4(\varepsilon_{ion}^{bare} - 1)}$$
$$- (1 + \varepsilon_{el}^{bare} - \varepsilon_{ion}^{bare})]. \tag{5b}$$

In Fig. 1, we plot $\varepsilon_{el}^{dressed}$ (top) and $\varepsilon_{ion}^{dressed}$ (bottom) as functions of $\varepsilon_{ion}^{bare}$, for the case where $\varepsilon_{el}^{bare} = 11$. We also plot the approximations that apply when $\varepsilon_{el} \gg \varepsilon_{ion}$ and when $\varepsilon_{el} \ll \varepsilon_{ion}$, extrapolated beyond their regions of validity. We see that for $\varepsilon_{ion}^{bare} \gtrsim 20$,[6] the "nearly-ferroelectric" approximation is rather good, while the "metallic" approximation is inapplicable.

In the present work, we employ the approximation [Eqs. (4a) and (4b)] that is valid for $\varepsilon_{ion} \gg \varepsilon_{el}$, since we deal with a very large $\varepsilon_{ion}$, and except at very small $q$ values, $\varepsilon_{el}$ is considerably smaller. The $q$ values that we are interested in are $q > q_D/3$, roughly, so that $\varepsilon_{el} < 10$. For very small $q$ values, the electron-ion matrix element $I$, which is proportional to $qV(q)$, is small; moreover, the volume in $k$ space of the regions with very small $q$ values is small; therefore, we are not concerned with them in this work. Thus, we regard the

electrons as being immersed in an ionic dielectric medium, and not the other way around, as is conventional in a "metallic" picture.

Our $\varepsilon_{ion}^{bare}$ is the dielectric constant of the insulating phase that is "close" to the superconducting, metallic phase; i.e., $YBa_2Cu_3O_6$ (or even $YBa_2Cu_3O_{6.5}$) for $YBa_2Cu_3O_7$; insulating phases of organic metals;[7] insulating $WO_3$ that is "close" to Na-doped $WO_3$.[8] This is in contrast with the Bohm-Pines-Nozières theory, where $\varepsilon_{ion}^{bare}$ involves a homogeneous plasma of ions, where the bare "phonon" frequency is the ion plasma frequency. This is unphysical in real solids, and thus must be replaced by $\varepsilon_{ion}^{dressed}$, which describes the real acoustic phonons.

We claim that approximating $\varepsilon_{el}^{dressed}$ by $\varepsilon_{el}^{bare}$ for values of $q$ which are small, but not extremely small, e.g., $q \approx k_F/3$, and values of $\omega$ smaller than $\omega_{trans}$, is unphysical for the nearly-ferroelectric metals, as illustrated in Fig. 1.

### III. CALCULATIONS

Consider a two-dimensional electron-gas sheet lying between two dielectric half-spaces as shown in Fig. 2. The separation between the dielectrics and the sheet is $d$. The dielectrics have a spatial periodicity in the $x$ and $y$ directions described by the susceptibility $\chi(\mathbf{r}_1)$, where $\mathbf{r}_1 = x\hat{i} + y\hat{j}$. The polarization vector $\mathbf{P}(\mathbf{r}_1, z)$ is related to the electric field $\mathbf{E}(\mathbf{r}_1, z)$,

$$\mathbf{P}(\mathbf{r}_1, z) = \chi(\mathbf{r}_1)\mathbf{E}(\mathbf{r}_1, z)[\Theta(z - d) + \Theta(-z - d)]$$
$$+ \delta(z) \int \chi_m(\mathbf{r}_1 - \mathbf{r}_1')\mathbf{E}_1(\mathbf{r}_1', 0)d\mathbf{r}_1', \tag{6}$$

where $\chi_m(\mathbf{r}_1)$ is the sheet susceptibility for the two-dimensional electron gas. Here $\Theta(z)$ is a unit step function.

Place a point test charge $Q$ at the position $\mathbf{r} = (\mathbf{R}, 0)$ so that the charge density is $\rho(\mathbf{r}_1, z) = Q\delta(\mathbf{r}_1 - \mathbf{R})\delta(z)$. The electric field may be expressed as the gradient of an electrostatic potential $\mathbf{E}(\mathbf{r}) = -\nabla V(\mathbf{r})$. By symmetry, $V(\mathbf{r}_1, -z) = V(\mathbf{r}_1, z)$. The susceptibility is taken to be a periodic function along the $x$ and $y$ directions, so

$$\chi(\mathbf{r}_1) = \sum_{\mathbf{G}} \chi_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}_1}, \tag{7}$$

where $\{\mathbf{G}\}$ are a set of two-dimensional reciprocal-lattice vectors.

For $z \neq 0$ and $z \neq \pm d$ the potential is a solution of the Laplace equation and may be expressed as

$$V(\mathbf{r}_1, z) = \int d^2 q_1 e^{\mathbf{q} \cdot \mathbf{r}_1}[f(\mathbf{q}_1)e^{-q_1 z}\Theta(z - d) + [g(\mathbf{q}_1)e^{-q_1 z}$$
$$+ h(\mathbf{q}_1)e^{q_1 z}]\Theta(z)\Theta(d - z) + [g(\mathbf{q}_1)e^{q_1 z}$$
$$+ h(\mathbf{q}_1)e^{-q_1 z}]\Theta(-z)\Theta(d + z)$$
$$+ f(\mathbf{q}_1)e^{q_1 z}\Theta(-z - d)]. \tag{8}$$

The Poisson equation for the transverse-Fourier-transformed electric field $\mathbf{E}(\mathbf{q}_1, z)$ and polarization field $\mathbf{P}(\mathbf{q}_1, z)$ becomes
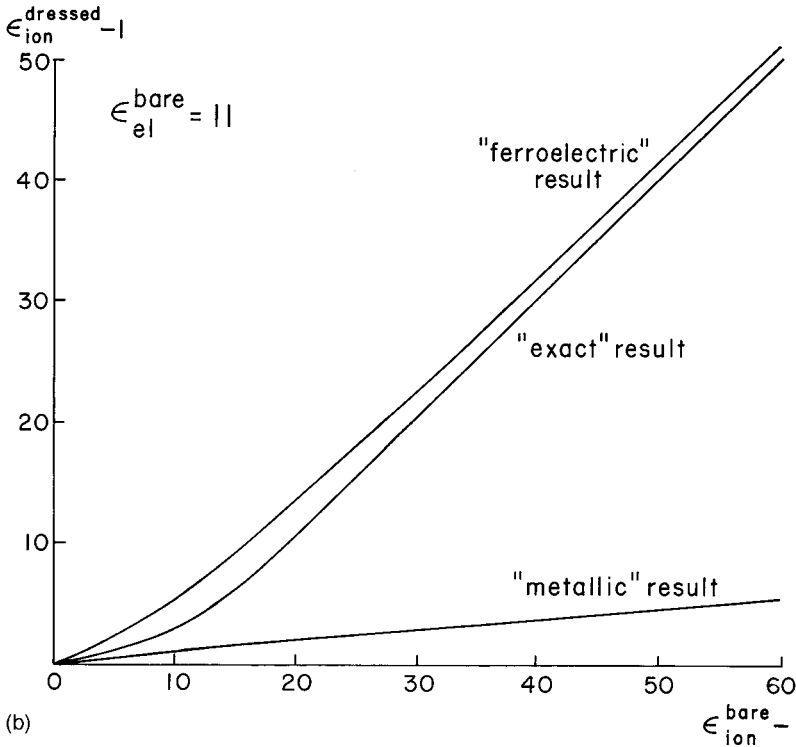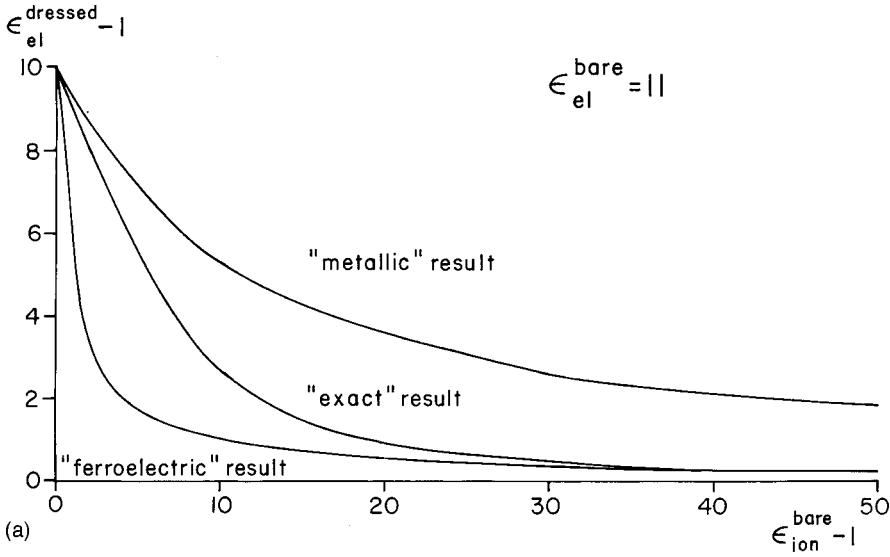
FIG. 1. The dressed dielectric constants $\varepsilon_{el}^{dressed}$, $\varepsilon_{ion}^{dressed}$ as a function of $\varepsilon_{ion}^{bare}$, for $\varepsilon_{el}^{bare} = 11$. We plot the exact values, as well as the approximate values that apply when $\varepsilon_{el}^{bare} \gg \varepsilon_{ion}^{bare}$ ("metallic" approximation) and $\varepsilon_{ion}^{bare} \gg \varepsilon_{el}^{bare}$ ("nearly ferroelectric approximation").

$$\frac{\partial E_z}{\partial z} + 4\pi\frac{\partial P_z}{\partial z} + i\mathbf{q}_1 \cdot (\mathbf{E}_1 + 4\pi\mathbf{P}_1) = \frac{Q}{\pi}\delta(z)e^{-i\mathbf{q}_1\cdot\mathbf{R}}. \quad (9)$$

Continuity of the normal component of the electric displacement vector at $z = d$ gives

$$q_1 f(\mathbf{q}_1)e^{-q_1 d} + \sum_{\mathbf{G}} 4\pi\chi_{\mathbf{G}}|\mathbf{q}_1 - \mathbf{G}|f(\mathbf{q}_1 - \mathbf{G})e^{-|\mathbf{q}_1 - \mathbf{G}|d}$$

$$= q_1 g(\mathbf{q}_1)e^{-q_1 d} - q_1 h(\mathbf{q}_1)e^{q_1 d}$$

and at $z = 0$ gives

$$2q_1[g(\mathbf{q}_1) - h(\mathbf{q}_1)] + 4\pi i\chi_m(\mathbf{q}_1)\mathbf{q}_1\cdot\mathbf{E}_1(\mathbf{q}_1,0) = \frac{Q}{\pi}e^{-i\mathbf{q}_1\cdot\mathbf{R}}.$$

Continuity of the potential at $z = d$ gives

$$f(\mathbf{q}_1)e^{-q_1 d} = g(\mathbf{q}_1)e^{-q_1 d} + h(\mathbf{q}_1)e^{q_1 d}.$$

The potential in the plane $z = 0$ is

$$V(\mathbf{r}_1) = \int d^2 r_1 e^{i\mathbf{q}_1\cdot\mathbf{r}_1}[g(\mathbf{q}_1) + h(\mathbf{q}_1)].$$

The solution proceeds as follows. Let $\Lambda(\mathbf{q}_1) \equiv [Q/(2\pi q_1)]\exp(-i\mathbf{q}_1\cdot\mathbf{R})$, so

$$\begin{bmatrix} 1 + 2\pi q_1\chi_m & -1 + 2\pi q_1\chi_m \\ 1 & e^{2q_1 d} \end{bmatrix}\begin{bmatrix} g \\ h \end{bmatrix} = \begin{bmatrix} \Lambda \\ f \end{bmatrix}.$$

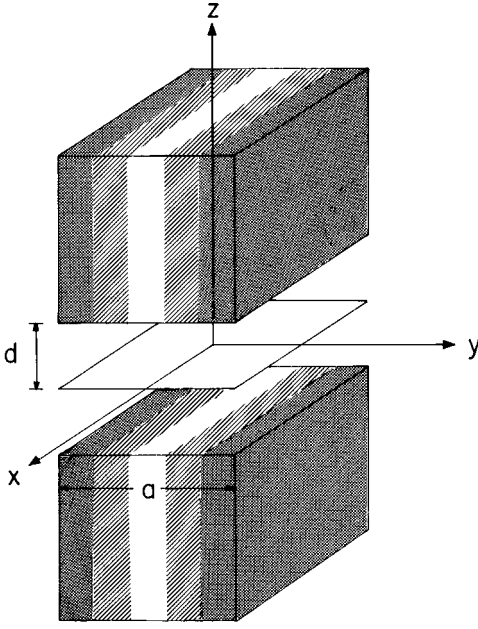Solving for $g$ and $h$ in terms of $f$ yields

FIG. 2. The configuration of the dielectrics and 2D metallic sheet employed in the present calculation. The darkness of the shading of the dielectrics illustrates the strength of the local dielectric constant. The dielectric is to be extended periodically in the x-y plane. In the figure, we illustrate modulation in the y direction. In the calculation, modulation in the x direction is considered as well.

$$g = \frac{\Lambda e^{2q_1 d} + (1 - 2\pi q_1 \chi_m)f}{\Delta} \qquad (10a)$$

and

$$h = \frac{-\Lambda + (1 + 2\pi q_1 \chi_m)f}{\Delta}, \qquad (10b)$$

where $\Delta = (1 + 2\pi q_1 \chi_m)\exp(2q_1 d) + 1 - 2\pi q_1 \chi_m$ is the determinant of the matrix.

One obtains an infinite set of coupled algebraic equations for the set of functions $\{f(\mathbf{q}_1 - \mathbf{G})\}$,

$$\sum_{\mathbf{G}''} M_{\mathbf{G}'\mathbf{G}''}(\mathbf{q}_1)f(\mathbf{q}_1 - \mathbf{G}'') = \eta_{\mathbf{G}'}(\mathbf{q}_1), \qquad (11)$$

where

$$M_{\mathbf{G}'\mathbf{G}''}(\mathbf{q}_1) = [1 + 2\pi|\mathbf{q}_1 - \mathbf{G}'|\chi_m(\mathbf{q}_1 - \mathbf{G}')]\delta_{\mathbf{G}'\mathbf{G}''}$$

$$+ \frac{4\pi}{|\mathbf{q}_1 - \mathbf{G}'|}[\cosh|\mathbf{q}_1 - \mathbf{G}'|d + 2\pi|\mathbf{q}_1 - \mathbf{G}'|$$

$$\times \chi_m(\mathbf{q}_1 - \mathbf{G}')\sinh|\mathbf{q}_1 - \mathbf{G}'|d]\chi_{\mathbf{G}'' - \mathbf{G}'}|\mathbf{q}_1 - \mathbf{G}''|$$

$$\times e^{-|\mathbf{q}_1 - \mathbf{G}''|d}$$

and

$$\eta_{\mathbf{G}}(\mathbf{q}_1) = \frac{Qe^{-i(\mathbf{q}_1 - \mathbf{G}) \cdot \mathbf{R}}}{2\pi|\mathbf{q}_1 - \mathbf{G}|}.$$

The linear set of equations expressed as $M \cdot f = \eta$ is readily solved to give $f = M^{-1}\eta$. The Fourier-transformed potential in the plane $z = 0$ is

$$V(\mathbf{q}_1, 0) = \frac{\Lambda(e^{2q_1 d} - 1) + 2f}{\Delta}. \qquad (12)$$

The sheet susceptibility for the two-dimensional electron gas $\chi_m = \chi_1 + i\chi_2$ is given by the expressions[9]

$$\chi_1 = S[2\tilde{q} - C_-\sqrt{(\tilde{q} - u)^2 - 1} - C_+\sqrt{(\tilde{q} + u)^2 - 1}] \qquad (13a)$$

and

$$\chi_2 = S[D_-\sqrt{1 - (\tilde{q} - u)^2} - D_+\sqrt{1 - (\tilde{q} + u)^2}], \qquad (13b)$$

where $C_\pm = \mathrm{sgn}(\tilde{q} \pm u)\Theta(|\tilde{q} \pm u| - 1)$, $D_\pm = \Theta(1 - |\tilde{q} \pm u|)$, $S = Ne^2/[m^*\tilde{q}(q_1 v_F)^2]$, $\tilde{q} = q_1/(2k_F)$, $v_F = \hbar k_F/m^*$, and $u = \omega/(q_1 v_F)$. Here $N$ is the number of electrons per unit area, and the Fermi wave-vector is given by $k_F = \sqrt{2\pi N}$. Atomic units are used in which $e = \hbar = m^* = 1$.

In the calculations a simple sinusoidal form for the dielectric susceptibility was employed

$$\chi = \frac{\varepsilon_1 - 1}{4\pi} + \frac{\varepsilon_2}{8\pi}\left[\cos\frac{2\pi x}{a} + \cos\frac{2\pi y}{a}\right]. \qquad (14)$$

### Approximations

We should note here two important approximations made in this calculation. First, we use the susceptibility $\chi_m(q_1)$ of an unperturbed free-electron gas, given by Ando, Fowler, and Stern.[9] Second, we assume that the dielectric susceptibility of the insulator, $\chi(r_1)$, is local in $\mathbf{r}$ space, i.e., $\mathbf{D}(\mathbf{r}) = \varepsilon_{\mathrm{ion}}(\mathbf{r})\mathbf{E}(\mathbf{r})$.

### IV. RESULTS

The main result of the paper is given in Eq. (12), which gives the Fourier transform of the potential in the conducting plane. The quantities $\Lambda$, $\Delta$, and $f$ are defined in Sec. III in terms of the parameters of the model. In limiting cases the results assume a much simpler form, as given below.

In the absence of the dielectric half spaces and without electron screening in the $z = 0$ plane the interaction potential set up by a point charge located at position $(\mathbf{R}, 0)$ is simply $V(\mathbf{r}) = Q/\sqrt{(\mathbf{r}_1 - \mathbf{R})^2 + z^2}$. The Fourier expansion of this is

$$V(\mathbf{r}_1, z) = \int d^2 q_1 f(\mathbf{q}_1)e^{i\mathbf{q}_1 \cdot \mathbf{r}_1 - q_1|z|},$$

where

$$f(\mathbf{q}_1) = \frac{Qe^{-i\mathbf{q}_1 \cdot \mathbf{R}}}{2\pi q_1}.$$

This (without the exponential) is plotted for reference purposes in Fig. 3(a) as curve (i). The location of the point charge $Q$ is taken to be at the origin and is given a unit strength.
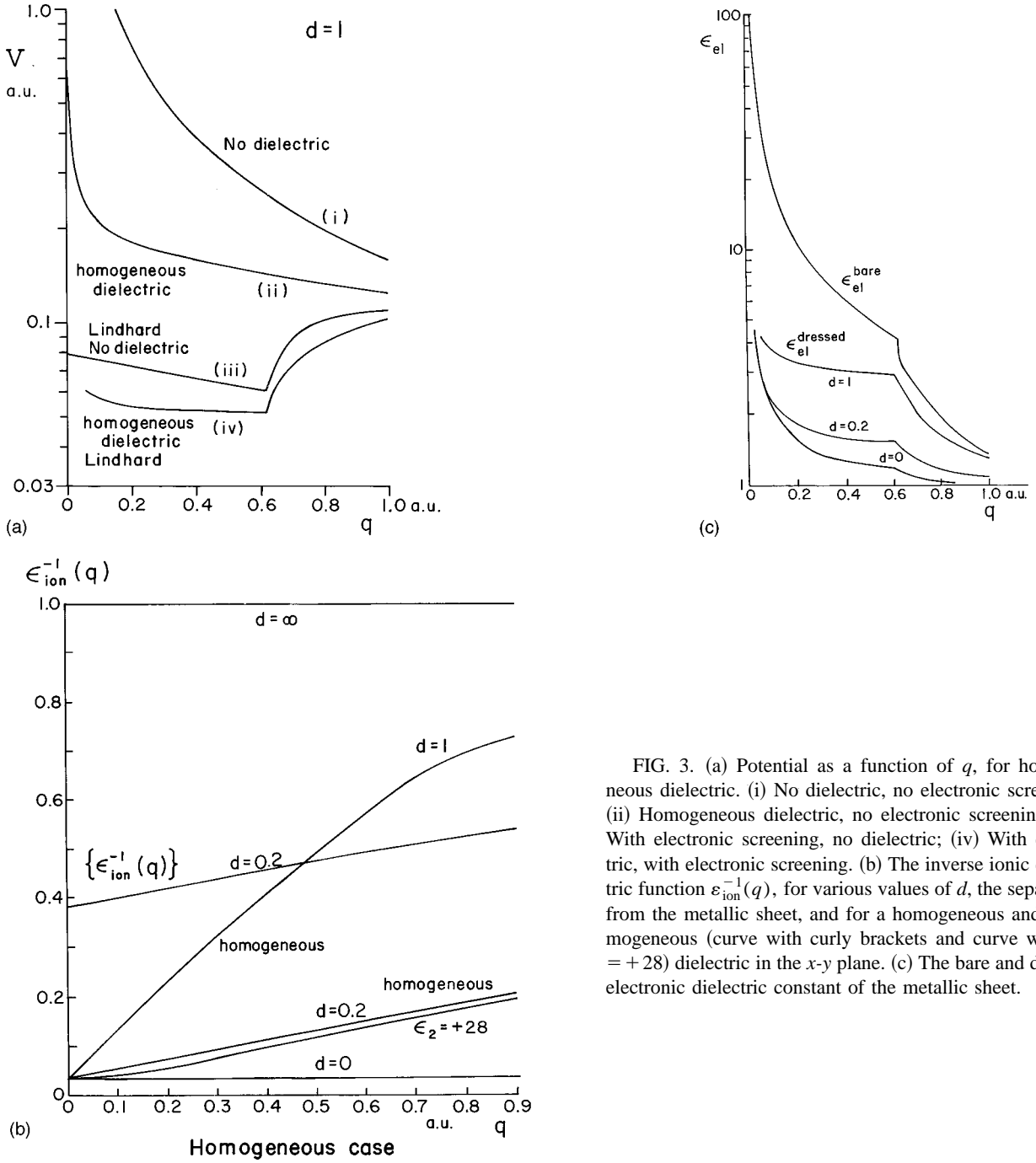
(a)



(b)



(c)

FIG. 3. (a) Potential as a function of $q$, for homogeneous dielectric. (i) No dielectric, no electronic screening; (ii) Homogeneous dielectric, no electronic screening; (iii) With electronic screening, no dielectric; (iv) With dielectric, with electronic screening. (b) The inverse ionic dielectric function $\varepsilon_{ion}^{-1}(q)$, for various values of $d$, the separation from the metallic sheet, and for a homogeneous and inhomogeneous (curve with curly brackets and curve with $\varepsilon_2 = +28$) dielectric in the $x$-$y$ plane. (c) The bare and dressed electronic dielectric constant of the metallic sheet.

In the absence of a dielectric (i.e., $\chi_1 = 0$) the Fourier transform of the potential assumes the form

$$V(q_1, z=0) = \frac{Q}{2\pi q_1} \frac{e^{-i\mathbf{q}_1 \cdot \mathbf{R}}}{1 + 2\pi q_1 \chi_m(q_1)}. \quad (15)$$

We can write this expression as

$$V(q_1, z=0) = \frac{Q}{2\pi} \frac{e^{-i\mathbf{q}_1 \cdot \mathbf{R}}}{q_1 + a_0^{-1}}, \quad (15a)$$

where $a_0 = \hbar^2 \varepsilon_\infty / m_* e^2$. This expression applies as long as $q_1 < 2k_F$. The effect of the electronic screening is simply to renormalize the charge $Q$ by a wave-vector-dependent

screening factor. This is plotted in Fig. 3(a), curve (iii). It can be seen to suppress the potential for small values of $q_1$ and to introduce the Fermi-level discontinuity in slope at $2k_F$.

In Fig. 3(a), curve (ii), the homogeneous dielectric half spaces are introduced. The values of the dielectric constant parameters were taken to be $\varepsilon_1 = 30$ and $\varepsilon_2 = 0$. The distance from the $z=0$ plane to the half spaces, $d$, is taken to be 1 atomic unit. One notes a substantial reduction of the interaction potential as a function of $q_1$.

The dielectric response function $\varepsilon_{ion}^{-1}(q)$ is defined as[10a] $V(q) = V_0(q) \varepsilon_{ion}^{-1}(q)$, where $V_0(q)$ is the potential without the dielectric, and $V(q)$ is the potential with the dielectric. For a dielectric uniform in the $x$-$y$ plane, i.e., $\varepsilon_2 = 0$, this

definition is straightforward. In Fig. 3(b) we plot $\varepsilon_{\mathrm{ion}}^{-1}(q)$ as a function of $q$, for $d=1$ and $d=0.2$. We see that when $q \to 0$, $\varepsilon_{\mathrm{ion}}^{-1}(q) \to \varepsilon_1^{-1}$, and when $q \to \infty$, $\varepsilon_{\mathrm{ion}}^{-1}(q) \to 1$. The crossover occurs when $q < d^{-1}$. Because of the very large value of $\varepsilon_1$, when $q$ is about one order of magnitude less that $d^{-1}$, $\varepsilon_{\mathrm{ion}}^{-1}(q)$ is already significantly larger than $\varepsilon_1^{-1}$.

The electronic dressed dielectric constant [Eq. (4)] is given by the Lindhard 2D screening in the $z=0$ plane:[9]

$$\varepsilon_{\mathrm{el}}^{\mathrm{dressed}}(q_1) = 1 + 2\pi q_1 \chi_m(q_1) \varepsilon_{\mathrm{ion}}^{-1}(q_1). \qquad (16)$$

We plot $\varepsilon_{\mathrm{el}}$ in Fig. 3(c). Thus, we can write

$$V(q_1, z=0) = \frac{Q}{2\pi} \frac{e^{i\mathbf{q}_1 \cdot \mathbf{R}}}{q_1 + a_0^{-1} \varepsilon_{\mathrm{ion}}^{-1}(q_1)}. \qquad (16a)$$

The screening length is seen to be $a_0[\varepsilon_{\mathrm{ion}}^{-1}(q_1)]^{-1}$. We plot the potential $V(q_1) = f(q_1)/\varepsilon_{\mathrm{el}}^{\mathrm{dressed}}(q_1)$ in Fig. 3(a) (iii), for the case without a dielectric ($\varepsilon_{\mathrm{ion}} = 1$), and in Fig. 3(a) (iv) for the case $\varepsilon_{\mathrm{ion}}^{\mathrm{bare}} = 30$.

The electron areal density was taken to be $N = 1/a^2$, corresponding to one free electron per unit cell. The effective mass of the electron was taken to be 1, and $a = 8$ a.u.

Comparing curves (i) and (iii) of Fig. 3(a), one sees that the Lindhard screening strongly suppresses the magnitude of the interaction potential, as would be expected. It leads to a finite value at $q_1 = 0$ and introduces a discontinuity in slope at $q_1 = 2k_F$. For values of $q_1$ larger than $2k_F = 0.627$ a.u., corresponding to short distances in configuration space, the electron sea becomes less effective in screening and hence there is a slight rise in the interaction potential.

When $q_1$ is extremely small, $\varepsilon_{\mathrm{el}}(q_1)$ is seen to be very large. For that case the approximation of Eq. (4) is not valid, and we should employ Eq. (3) (Sec. II). In the present work we are not concerned with that region.

When $q_1$ is small, but not extremely small, $q_1 \chi_m(q_1)$ varies as $q_1^{-1}$, and $\varepsilon_{\mathrm{ion}}^{-1}(q_1)$ increases linearly with $q_1$, thus $\varepsilon_{\mathrm{el}}^{\mathrm{dressed}}(q_1)$ is approximately constant [Fig. 3(c)]. This is the region that interests us in the present work. In this region, $\varepsilon_{\mathrm{ion}}^{-1}(q_1)$ in the numerator and denominator cancel each other, and the potential is close to that without a dielectric altogether. We show this in Fig. 3(a), curve (iv), which is only slightly lower than Fig. 3(a), curve (iii).

When $q_1$ gets larger $\varepsilon_{\mathrm{el}}^{\mathrm{dressed}}(q_1)$ falls rapidly and the screening of the potential by the conduction electrons is no longer important.

Thus, the results for a dielectric homogeneous in the $x$-$y$ plane are what is to be expected.

### Inhomogeneous case

We now introduce inhomogeneity into the dielectric half spaces. The size of the inhomogeneity is determined by the numerical values of the constants $\varepsilon_1$ and $\varepsilon_2$. They are taken to be 30 and $-28$, respectively. Thus, in a unit cell the dielectric constant varies from as much as $\varepsilon_1 - \varepsilon_2$, or 58, to as little as $\varepsilon_1 + \varepsilon_2$, or 2. The size of the unit cell is taken to be $a = 8$ a.u.

When the dielectric is inhomogeneous in the $x$-$y$ plane, i.e., $\varepsilon_2 \neq 0$ and is large, the situation changes radically from the homogeneous case. Since the system is inhomogeneous, the potential at point $\mathbf{r} + \mathbf{R}$ due to a charge at point $\mathbf{R}$ now depends not only on the distance $r$, but it depends on $\mathbf{R}$ explicitly, and in a strong way. We denote the dielectric response function due to a unit charge at point $\mathbf{R}$ by $\varepsilon^{-1}(\mathbf{q}; \mathbf{R})$. Since the lattice is periodic, $\varepsilon^{-1}$ is periodic in $\mathbf{R}$. The dielectric response is now represented by a tensor. This tensor, in the form of its Fourier transform $\varepsilon^{-1}(\mathbf{q} + \mathbf{G}, \mathbf{q} + \mathbf{G}')$, was introduced and treated in some detail in the past.[10] In this case $q$ is replaced by $q_1$; because of the inhomogeneity, there is a difference between the [100] and [110] directions; however, this difference is small and we ignore it here. When we choose $R = 0$, i.e., the minimum value of $\varepsilon(\mathbf{R})$, we denote the dielectric response function by the curly brackets: $\{\varepsilon_{\mathrm{ion}}^{-1}(q)\}$. We plot $\{\varepsilon_{\mathrm{ion}}^{-1}(q)\}$ in Fig. 3(b) for $\varepsilon_1 = 30$, $\varepsilon_2 = -28$, $d = 0.2$. (We employ different types of brackets, namely, square, triangular, and curly ones, to denote the different types of averages). We define the various averages in terms of the inverse dielectric tensor $\varepsilon^{-1}(q + G, q + G')$ in another publication[10b].

In Fig. 3(b) the effect of location of the inhomogeneous dielectric half spaces is studied by assigning the value $\varepsilon_2 = +28$ instead of $-28$. This effectively shifts the lattice by half a lattice constant, interchanging the maxima and minima of the dielectric constant. It is seen that this curve is close to the homogeneous case. For the $\varepsilon_2 = +28$ curve, the high dielectric constant regions lie close to the location of the charge, so there is a strong screening effect. For the $\{\varepsilon_{\mathrm{ion}}^{-1}\}$ curve the low dielectric regions lie close to the location of the charge and so have only a slight effect on the interaction potential.

The average inverse dielectric function is given by

$$\langle \varepsilon_{\mathrm{ion}}^{-1}(0) \rangle = \frac{1}{a^2} \int_0^a dx \int_0^a dy \, \frac{1}{\varepsilon_1 + \dfrac{\varepsilon_2}{2}\left[\cos\dfrac{2\pi x}{a} + \cos\dfrac{2\pi y}{a}\right]}. \qquad (17)$$

For our parameters, $\langle \varepsilon_{\mathrm{ion}}^{-1}(0) \rangle^{-1} = 19.2$, while $\langle \varepsilon_{\mathrm{ion}} \rangle = 30$. The difference between $\langle \varepsilon^{-1} \rangle^{-1}$ and $\langle \varepsilon \rangle$ is not very large. For a modulation in one direction only, i.e., $\varepsilon(x) = \varepsilon_1 + \varepsilon_2 \cos(2\pi x/a)$, the difference is larger and $\langle \varepsilon_{\mathrm{ion}}^{-1}(0) \rangle^{-1}$ is given by $\sqrt{2\varepsilon_{\mathrm{min}}\langle\varepsilon\rangle} \approx 11$.

Since $\varepsilon_{\mathrm{ion}}^{-1}(\mathbf{q}; \mathbf{R})$ depends on the position $\mathbf{R}$ of the charge, we have to average over $\mathbf{R}$ to obtain the ionic dielectric response function of the *electron gas*. For the uniform electron gas that we consider here,

$$[\varepsilon_{\mathrm{ion}}^{-1}(q)] = \frac{1}{a^2} \int_0^a dx \int_0^a dy \, \varepsilon_{\mathrm{ion}}^{-1}(\mathbf{q}; \mathbf{R}). \qquad (18)$$

We denote this average using square brackets. We calculated the average over $\mathbf{R}$ numerically, by taking the average over 24 points in the unit cell. The peak of $\varepsilon_{\mathrm{ion}}^{-1}(\mathbf{q}; \mathbf{R})$ around $\mathbf{R} = 0$ is found to be very narrow. As $q \to 0$, $[\varepsilon_{\mathrm{ion}}^{-1}(0)]$ attains
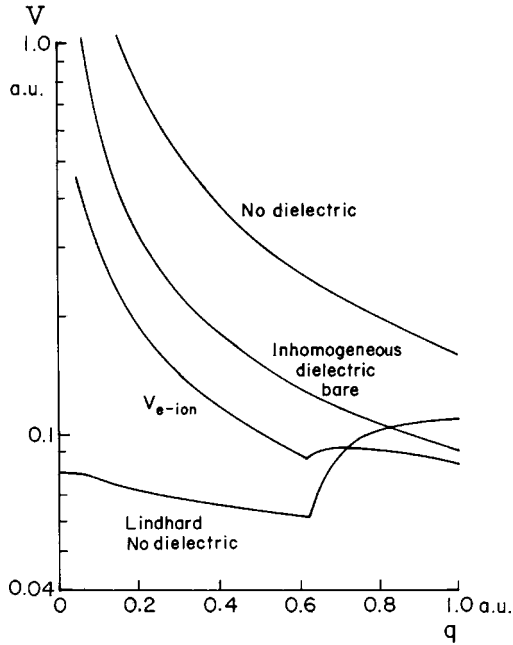
FIG. 4. The potential $V$ for an inhomogeneous dielectric, and the potential $V_{e\text{-ion}}$ screened by the conduction electrons. The potential without the dielectric (without and with electronic screening) are also replotted. The electronically screened potential with the dielectric is considerably stronger than the potential without the dielectric for small $q$ values.

(nearly) the same value as $\langle \varepsilon_{ion}^{-1}(0) \rangle$, since in both cases we have to average over the whole space. As $q \to \infty$, $[\varepsilon_{ion}^{-1}(q)] \to 1$, since $d$ is finite. For values of $q$ that are small, but not very small, i.e., $q \approx a^{-1}$, $[\varepsilon_{ion}^{-1}(q)]$ differs from $\{\varepsilon_{ion}^{-1}(q)\}$ by a very large amount—it is much smaller. The reason is that $\varepsilon_{ion}^{-1}(q)$ approaches the *local* value of $\varepsilon^{-1}(\mathbf{R})$ at $R = 0$ which is very large [0.5 for our parameters, where $\varepsilon(0) = 2$]. On the other hand, $[\varepsilon_{ion}^{-1}(q)]$ is an average over $\mathbf{R}$ even for finite $q$, and since the average $\varepsilon_{ion}(\mathbf{R})$ is so much larger than the minimum (30 vs 2), the average of $\varepsilon_{ion}^{-1}$ is so much smaller.

Our result that $\{\varepsilon_{ion}^{-1}(0)\}$ is so much larger than $[\varepsilon_{ion}^{-1}(0)] \approx \langle \varepsilon_{ion}^{-1}(0) \rangle$ is the result of our assumption that the dielectric is extended in the $z$ direction (to $\pm\infty$, in our model). The experimental infrared results[6] substantiate this assumption; the measured dielectric constant is the average over $z$. If the dielectric would extend only a small distance (of order 1 a.u.) in the $z$-direction, the measured average would be much smaller.

For the inhomogeneous case, the electronic dielectric function is given by Eq. (16), with $\varepsilon_{ion}^{-1}(q_1)$ replaced by $[\varepsilon_{ion}^{-1}(q_1)]$.

We plot the potential $V_{el\text{-ion}}(q)$, which takes into account both the dielectric screening and the screening by the conduction electrons $\varepsilon_{el}^{dressed}$, in Fig. 4. The result that we find is striking. The potential $V_{el\text{-ion}}(q)$ is considerably *stronger* for small $q$ values than the potential without the dielectric. For $q = 0.12$ a.u. $= q_{stripe}$ (Ref. 11) the enhancement is by more than a factor of 3. The effect of the conduction electrons (which reduce $V$) is reduced by the inhomogeneous dielectric

much more than the potential itself; thus we have an effect of strong *overscreening*. Writing (qualitatively) $\{\varepsilon_{ion}^{-1}\} \to \varepsilon_{local}^{-1}$, $[\varepsilon_{ion}^{-1}] \to \varepsilon_{average}^{-1}$, we obtain

$$V_{el\text{-ion}} \approx V_{homogeneous} \frac{\varepsilon_{local}^{-1}}{\varepsilon_{average}^{-1}}, \tag{19}$$

where $V_{homogeneous}$ denotes the potential without the dielectric, but with the electronic screening in a homogeneous system, given (at $q = 0$) by $V_{homogeneous} = Z/N(0)$.[12] [In two dimensions, $N(0) = m^*/(\pi\hbar^2) = (\pi e^2 a_0)^{-1}$].

## V. ROLE OF THE SPECIFIC PARAMETERS

The effect that we describe here, namely, a large *overscreening* of the electron-ion potential by the inhomogeneous dielectric, which increases the value of this potential by a large factor, depends in a critical way upon the specific values of the parameters, namely, the ionic dielectric constant $\varepsilon$, the scattering wave vector $q$, the distance between the dielectric and the metallic sheet $d$, the average distance between the conduction electrons $a$, and the extension of the dielectric in the $z$ direction (infinite in our model). The effect is present only for a rather restricted range of values of these parameters, and for $\omega < \omega_{trans} \approx 19$ meV (in the cuprates).

The strength of the potential $V(q)$ depends on $\varepsilon_{ion}$ up to $\varepsilon_{ion} \approx 20$, and for larger values of $\varepsilon_{ion}$ it saturates. For $q = 0.6$ a.u. there is still an effect, but it is much smaller, and for $q = 1$ a.u. $V(q)$ is almost independent of $\varepsilon_{ion}$. The value $q = 0.12$ a.u. is roughly $k_P/3$, thus to get a large effect $q$ must be small, but not very small, and $\varepsilon_{ion}$ should be about 20 or 30. For values of $\varepsilon_{ion}$ typical of nonferroelectric oxides, namely, $\varepsilon_{ion} \approx 3-4$, the effect is small. For very large values of $\varepsilon_{ion}$, namely, about 100 or more, we do not gain much, but being close to the ferroelectric transition, we risk instabilities; in the ferroelectric state, the interaction weakens.[13]

The depth of the modulation of the dielectric constant must be extremely large. We take $\varepsilon_{ion}^{min} = 2$, $\varepsilon_{ion}^{average} = 30$, and $\varepsilon_{ion}^{max} = 58$. This is based on the assumption that the large observed dielectric constant of the cuprates is due to the apex oxygen atoms and the alkaline-earth atoms, and the polarizability of the planar oxygen is small.

When $q$ is very small (about $k_F/10$ or so), $\varepsilon_{el}^{bare}$ exceeds $\varepsilon_{ion}^{bare}$, and our approximation is not valid (see Sec. II). In that case, $\varepsilon_{ion}$ is screened out by $\varepsilon_{el}$ and $V(q)$ is not greatly affected by the dielectric.

The role of the separation $d$ is somewhat subtle. Naively we might expect that for a value of $q$ that is about one order of magnitude smaller that $d^{-1}$ the dielectric screening of both the electron-ion and the electron-electron potentials is about complete. This is not the case. In Fig. 5 we plot the potential $V(q)$ (without the screening by the conduction electrons) as a function of $q$ for $d = 1$ a.u. and $d = 0.2$ a.u., as well as the potential without the dielectric ($d \to \infty$). The potential for $d = 0.2$ a.u. is close to $V(q)/\varepsilon$ (i.e., a homogeneous dielectric in all space), except for very large $q$ values. We see that for *very* small $q$ values, the potential for $d = 1$ a.u. is close to that for $d = 0.2$ a.u., while for large $q$ values, it is close to the potential without the dielectric. This
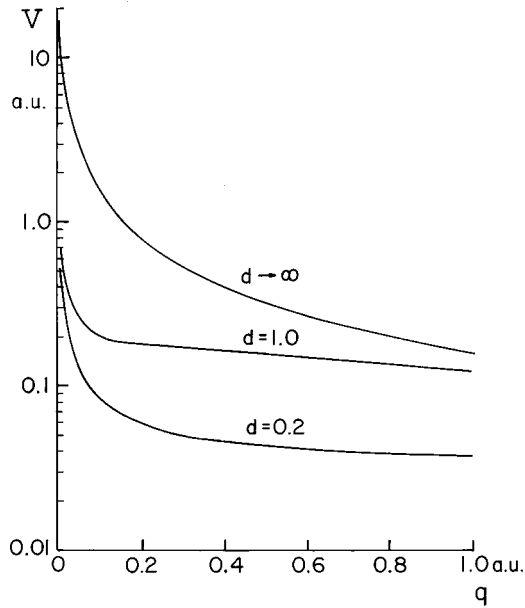
FIG. 5. The potentials (without electronic screening) for various values of the separation $d$ of the dielectric.

is what is to be expected. However, already at values of $q$ one order of magnitude less than $d^{-1}$, the potential is nearly an order of magnitude stronger than that for the $d=0.2$ a.u. case. This large increase in the small $q$ values ($q \approx 0.12$ a.u.) is (apparently) surprising.

The extension of the dielectric in the $z$ direction is also an important parameter. In the present calculation, we have considered half spaces extending to infinity. Let us denote this length of the dielectric by $L$. In Fig. 6 we illustrate the role of this parameter. In Fig. 6(a) we illustrate situations in which the dielectric is *not* very effective in screening out the potential at point $\mathbf{r}$ due to the charge $Q$. In configuration I, a dielectric between $Q$ and $\mathbf{r}$ is not effective, since the polarization charge $-Q$ on one side of the dielectric neutralizes $Q$, and $+Q$ on the other side produces a potential equal to that of $Q$. The same situation occurs when the separation $d$ is not zero. A spherical dielectric shell around $Q$ (in 3D or 2D), illustrated in configuration II, also does not screen out the potential due to $Q$ outside the shell. Dielectrics of length $L$, with $L<a$, are also not effective in screening out the potential (configuration III). In Fig. 6(b) we illustrate a dielectric constant with $L\gg a$. The charge $Q$ is situated in the space between the dielectrics, a distance $d$ away, where $d\ll a$. In this case, the dielectric is *effective* in screening out the potential due to the charge $Q$. In Fig. 6(c) we illustrate the group of atoms in YBCO that we consider as the "dielectric," namely, the apex oxygen, the chain copper (or Bi, Tl, Hg in other cuprates), and the next apex oxygen. Thus, $L$ is seen to be large. In the organic superconductors, the flat molecules are also long compared with the distance between adjacent molecules.

Thus, while the electron-ion potential (at the site of the planar oxygen) is not effectively screened by the dielectric for the inhomogeneous case, the electron-electron interaction
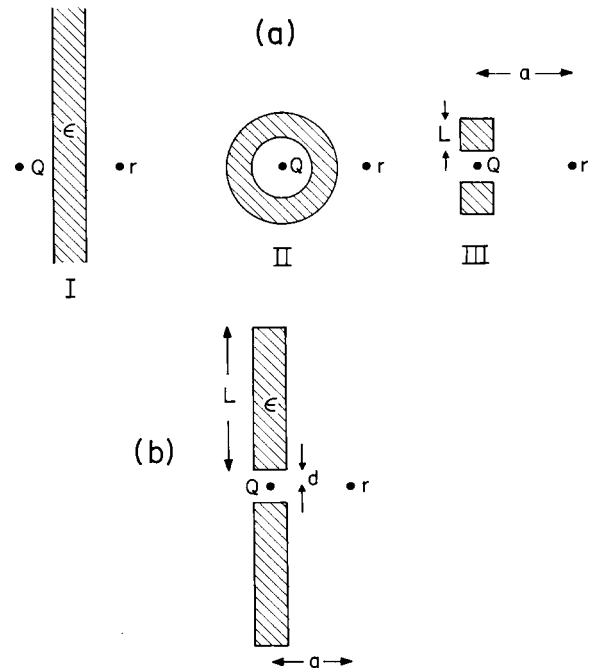


FIG. 6. Illustration of the configuration that gives rise to strong ionic screening of the electron-electron interaction. (a) Configurations that do not give much dielectric screening; (b) Configuration that is effective in providing dielectric screening; (c) The complex of atoms in $YBa_2Cu_3O_7$ that provides the dielectric screening.

that is the cause of the Lindhard screening *is* effectively screened.

We see that to obtain the effect of overscreening, $d$ must be very small, of the order of a Bohr radius. For such short distances a "macroscopic" description is obviously not ap-

propriate and we need a microscopic, quantum-mechanical one. We shall discuss this later.

Thus, the effect that we describe here exists only over a narrow range of the parameters and therefore is rather elusive.

## VI. DISCUSSION

In a homogeneous system, the electron-ion potential $V_{el-ion}(q)$ at $q = 0$ is given by: $V_{el-ion} = Z/N(0)$. This rather general result[12] is the basis of McMillan's estimate of the maximum $T_c$ due to the phonon-mediated mechanism.[14] In an inhomogeneous system this result no longer holds.

We looked into two kinds of inhomogeneities: First, inhomogeneity in the $z$-direction. We consider a dielectric separated from an infinitesimally thin metallic layer by a distance $d$. Second, we consider an inhomogeneous dielectric in the $x$-$y$ plane, with a periodic in-plane variation of the dielectric constant with a lattice constant $a$.

The first kind of inhomogeneity does not increase $V_{el-ion}(q)$ above the value without a dielectric. Actually, $V_{el-ion}(q)$ for small $q$ values is reduced by about 20% by the dielectric (for characteristic parameters). This is not a big effect; without the electronic screening the potential is reduced by the dielectric by about 80%. The reason why the effect is small, is that the electronic screening is reduced by the dielectric to nearly the same extent as the bare potential, and the two effects nearly cancel. At large $q$ values, where the electronic screening is weak, the dielectric has little effect because $q$ is of order $d^{-1}$. Therefore, if we neglect the dielectric altogether, the error is very small. This may be the reason why conventional band structure calculations, which neglect the ionic dielectric constant altogether, give such good results.

The situation changes completely when the large inhomogeneity in the $x$-$y$ plane is introduced. The electron-ion potential is screened by the *local* value of the dielectric constant, while the electron-electron interaction is screened by the *average* value, and these two may differ greatly. As a result, we get a very large increase of the electron-ion potential.

The cause of this very large increase is that the electron-ion interaction is dominated by the potential at very short distances for small (but not extremely small) $q$ values. In contrast, the electron-electron interaction that causes electronic screening described by the Lindhard function is dominated by the electron-electron potential (shielded by the dielectric) at distances of order $r_s a_0$ ($a_0$ being the Bohr radius), which in our model are about $a = 8$ a.u. $\approx 4$ Å, ($a$ being the lattice constant in the cuprates). This distance is an order of magnitude larger than $d = 1$ a.u.; therefore the electron-electron interaction is shielded very effectively by the dielectric, while the electron-ion interaction is not.

Alternatively, we can say that the shielding by the conduction electrons, described by the Lindhard function, is dominated by the cutoff at $q = 2k_F$, which is small (about 0.6 a.u. for the parameters that we consider). Thus, the Fourier components of the potential that characterize the inhomogeneity, at the reciprocal lattice vectors that are large (the

smallest reciprocal lattice vector $G$ being about twice $2k_F$), are cut off, and the electron gas sees only the *average* (or homogeneous component) of the dielectric function.

Thus, we have an effect of "overscreening." The dielectric reduces the "bare" electron-ion potential by a factor of about 5 (for the parameters that we consider), while it reduces the screening by the conduction electrons by a factor of about 20; thus we obtain a net *increase* of the potential by a factor of about 4.

This increase in the potential causes a very large increase in the McMillan electron-phonon coupling parameter $\lambda$, since $\lambda$ is proportional to the square of the potential. Since this increase takes place only at small (but not very small) values of $q$, the average over $q$ is increased by *less* that the square of this value. The average over $q$ is different in 2D and 3D; in 2D small $q_1$ values contribute much more to the average than in 3D. Therefore the increase of $\lambda$ in 3D is not very large, while in 2D it is. An explicit (albeit crude) estimate of this dimensional effect is given in Ref. 3. Also, this increase takes place only at small frequencies $\omega$, below the dispersion frequency of the ionic dielectric constant $\omega_{trans}$. The superconducting transition temperature $T_c$ is proportional to $\sqrt{\lambda}$ (for $\lambda \geq 2$). Taking into account both the necessity to average over $q$ and the low cutoff frequency $\omega_{trans}$, we estimate an increase in $T_c$ by a factor of 2–3 in 2D, and a considerably smaller increase in 3D.

The large overscreening is a very special feature of the particular geometry, consisting of a very *thin* metallic layer and a very *thick* dielectric layer [large $L$, Fig. 6(c)]. (The metallic layer in the present work is infinitesimally thin in the $z$ direction, and the role of its actual width $2a_c$ was described in Ref. 3, where it is shown that $T_c$ is proportional to $1/2a_c$. In the present work we show that the separation $d$ between the metallic layer and the dielectric must also be extremely small for the overscreening to be large.)

In addition, the $T_c$ is suppressed by the Coulomb repulsion between conduction electrons, denoted by $\mu$. The effect of this Coulomb repulsion is reduced by the small cutoff of the electron-phonon interaction $\Omega_{phonon}$ to $\mu^* = \mu/[1 + \mu \ln(E_F/\Omega_{phonon})]$, as shown by Bogolyubov.[14a] For the cuprates, with $\hbar\Omega_{phonon} \approx 40$ meV, $E_F \approx 1$ eV, $\mu^*$ is about 0.2. In the present case, the bare $\mu$ is screened out by the ionic dielectric constant to $\tilde{\mu} = \mu[\varepsilon_{ion}^{-1}]$, which is very small ($\mu \approx 0.35$ for a typical dilute electron gas, $[\varepsilon_{ion}^{-1}] \approx 0.07$ [Fig. 3(b)]; thus $\tilde{\mu} \approx 0.025$, roughly). However, since the cutoff of $[\varepsilon_{ion}^{-1}(\omega)]$ is very small (given by $\omega_{trans}$), there is no further reduction by the Bogolyubov mechanism. Since $\tilde{\mu}$ is about an order of magnitude smaller than $\mu^*$, there is a considerable increase in $T_c$ due to this cause, namely, by a factor of 2–3. Considering both factors, we obtain a maximum $T_c$ due to the electron-phonon mechanism of about 200 K.[3]

The use of a macroscopic dielectric constant at length scales of order 1 a.u. is questionable. When the apex-oxygen $2p_z$ orbital (or hybridized $2s$-$2p_z$ orbital) overlaps appreciably with the conduction-electron orbitals (i.e., Cu $3d_{x^2-y^2}$) directly, or indirectly, via the Cu $3d_{z^2}$ orbital, we can say that the effective distance $d$ is essentially zero, and the effect is huge. When such an overlap is weak, then $d$ is about 1 A,

which is so large that the effect is weak. The question whether such an overlap is present cannot be determined by a calculation based on a solution of the Laplace equation, as we do here, but requires a quantum-chemical calculation. A quantum-chemical calculation was carried out by Kamimura, Nomua, and Sano.[15] They find that under certain conditions the effective Hubbard interaction of the conduction electrons $U_{eff}$ is reduced below the bare value $U_{bare}$ by a very large amount. Writing $U_{eff} = U_{bare} \langle 1/\varepsilon \rangle$, their value for $\langle 1/\varepsilon \rangle^{-1}$ is even larger than the value used in the present work. This large value depends on the nature of the atom on the other side of the apex oxygen, namely, the *chain* copper in YBaCuO (or, alternatively, Tl, Hg or Bi; atoms such as Zn or Cd do not cause this effect). This atom is situated at a distance of about 4 A from the $(CuO_2)_n$ plane [Fig. 6(c)]. In our calculation the overscreening effect is present only when the dielectric is extended in the $z$ direction. This requires the chain atom to play a role. The point of "action at a distance" is emphasized by Anderson.[16] Our model differs from his, but we believe that his insistence that an acceptable theory must account for this "action at a distance" is well taken.

The "basic" question that this work addresses is whether the phonons play a vital role in the superconductivity of "exotic" superconductors.[3,17]

There is no question that the magnetic mechanism of Pines and co-workers[17a] plays a crucial role in the superconductivity of the cuprates. Above $T_c$, the electron-electron interaction is very strong and a free-electron picture is not valid even close to the Fermi level, as the detailed IR work shows.[2,18] Only below $T_c$ is the electron-electron interaction below the pseudogap reduced significantly. However, this does not eliminate the possibility of an important role for the phonon mechanism. Recently, the work of Shen, Lanzara, and Nagaosa[19] points out an important role of the phonons, and the work of Pan *et al.*[20] points out the crucial role of inhomogeneity over a scale of a lattice constant. Together with the strong isotope effect in underdoped samples, the near-exclusive high-temperature superconductivity in the perovskites, in contrast to other magnetic oxides, the abnormally high $T_c$ in the organics, the (apparent) superconductivity at 90 K of Na-doped $WO_3$, there is substantial evidence for an important role for the phonon mechanism. This work shows the role played by the chain metal atom ("action at a distance"), as well as the apex oxygen. In this way, we show how a strongly enhanced phonon-mediated interaction can occur in nearly ferroelectric metals, such as the perovskites.

## VII. EXPERIMENTAL SUPPORT

The basic presumption of this calculation is that the complex consisting of two apex oxygens and a bismuth (or chain-copper) atom in between [Fig. 6(c)] has an enormously large dipole moment, which gives rise to the large measured ionic dielectric constant in the $c$ direction.[6] The oscillator strength of the $c$-axis polarized phonon modes associated with this cluster was calculated theoretically. For the TO mode at 233 cm$^{-1}$ in $La_2CuO_4$ the oscillator strength calculated by Cohen *et al.*[21] is 4.3, while the measured value is 15.4,[22] i.e., almost four times stronger. For the analogous

mode at 155 cm$^{-1}$ in $YBa_2Cu_3O_7$, the oscillator strength calculated by Cardona and co-workers[23] is 3.78, while the measured value is 10.2,[22] i.e., about three times stronger. The situation is even more striking for the LO mode at 499 cm$^{-1}$ in $La_2CuO_4$, where the calculated oscillator strength is 0.02,[2f] while the measured value is 0.31, i.e., about 15 times stronger.

We believe that the cause of the large discrepancy between the calculated and experimental oscillator strength is that the calculated values do not take into account the charge-transfer between the atoms in the cluster. Since the bismuth is in a mixed-valence state, and the copper $3d \rightarrow 4s$ excitation energy is low,[15] charge transfer between the apex oxygens via these atoms is easy, and this increases the dipole moment and thus the oscillator strength by an enormous amount. This is the cause of the exceedingly large measured dielectric constant.[6] We believe that the present calculation is the first that considers the effect of this enormous localized polarizability on the electronic properties.

It is frequently argued that the $c$-axis polarizability and the charge motion in the $a$-$b$ plane are decoupled. It is easy to see from elementary electrostatics that these two degrees of freedom are strongly coupled. Experimentally, the work of Reedyk and Timusk[24] shows that at frequencies where $\varepsilon_{cc}(\omega)$ has a minimum, i.e., $\text{Im}[1/\varepsilon_{cc}(\omega)]$ has a maximum, the conductivity $\sigma_{a-b}(\omega)$ in the $a$-$b$ plane has a minimum. This is the frequency of the LO mode, which affects the dielectric constant by the Lyddane-Sachs-Teller relation,

$$\varepsilon_{ion}(\omega) = \varepsilon_{ion}(\infty) \left( \frac{\omega^2 - \omega_{LO}^2}{\omega^2 - \omega_{TO}^2} \right),$$

where $\omega \approx \omega_{LO}$ and $\varepsilon_{ion}(\omega)$ has a minimum. The electron-electron interaction $e^2/\varepsilon_{ion}(\omega) r_{12}$ (as well as the electron-ion interaction) is not effectively screened by $\varepsilon_{ion}$, and therefore the stronger electron-electron interaction causes scattering that decreases $\sigma_{a-b}(\omega)$.

The main conclusion of this work is that the electron-electron interaction is effectively screened out by the ionic dielectric constant, while the bare electron-ion interaction is not. This paradoxical situation is due to the extreme inhomogeneity of the dielectric constant in the $a$-$b$ plane. This effect is demonstrated in a striking way by the STM measurements of Pan *et al.*[20] They measure a very strong potential, due to oxygen interstitials or vacancies, with a range of about 14 A (in the $a$-$b$ plane). The expected screening length is about 1 A.[25] In a 2D electron gas, the screening length is given by $a_0 \approx \hbar^2/m^* e^2 \approx 0.16$ A for $m^* \approx 3m_e$. The dielectric constant increases this to $a_0 \varepsilon_{ion} \approx 5$ A when $d=0$. The measured decrease in the potential for distances of $r_1 \approx 15$ A or more is in accord with such a screening length. (The potential for $r_1 \gg a_0 \varepsilon_{ion}$ should fall off like $1/r_1^3$.[9] Experimentally,[20] it falls off approximately like $1/r_1^{2.5}$ for $r_1 > 15$ A). On the other hand, a *uniform* dielectric constant of $\varepsilon = 30$ would reduce the potential drastically. Experimentally, the potential is very strong, as evidenced by its effect on the local density of states, and the pseudogap.

The nearly perfect screening of the electron-electron interaction by the dielectric, is a direct indication that the separation $d$ between the dielectric and the metallic region is very

small—essentially zero. The apex-oxygen and planar-copper orbitals overlap appreciably. This effect was demonstrated by the quantum-chemical calculation of Kamimura, Nomua, and Sano[15] that includes the effect of configuration interaction.

The strong electron-phonon interaction, which is the result of the enhanced electron-ion potential calculated in this work, is seen experimentally by the angle-resolved photoemission spectroscopy measurements of Shen, Lanzara, and Nagaosa[19] who observe a break in the electronic energy vs $k$ curve at the appropriate phonon frequency.

When the lattice periodicity is broken by interstitial oxygen ions, vacancies, dopants, etc., the unscreened long-range nature of the potential gives rise to strains much larger than in metals. These ferroelastic effects have been investigated in detail by Phillips and Jung[26] who record a multitude of experimental anomalies caused by filaments in the $c$ direction. These anomalies manifest themselves in IR spectroscopy, neutron diffraction, superconducting tunneling in the $c$-direction, etc. Unlike Phillips, we do not attribute the su-

perconductivity *per se* to these $c$-axis filaments, but to the periodic lattice. The present RPA (random-phase approximation) calculation for a periodic, extremely inhomogeneous lattice is thus a step toward investigation of ''real'' doped nonperiodic systems, where the RPA is no longer applicable.

Thus, we believe that the results of the present calculation are supported quantitatively by a number of recent experiments.

[1] J. I. Gersten and M. Weger, Physica B **225**, 33 (1996).

[2] A. V. Puchkov, D. N. Basov, and T. Timusk, J. Phys.: Condens. Matter **8**, 10 049 (1996).

[3] M. Weger, M. Peter, and L. P. Pitaevskii, Z. Phys. B: Condens. Matter **101**, 573 (1996).

[4] N. W. Aschcroft and N. B. Mermin, *Solid State Physics* (Holt Saunders, Philadelphia, 1976), pp. 515–518.

[5] M. Weger, Acta Phys. Pol. A **87**, 723 (1995).

[6] J. Kircher, R. Henn, M. Cardona, P. L. Richards, and G. P. Williams, J. Opt. Soc. Am. B **14**, 705 (1997); R. Henn, A. Wittlin, M. Cardona, and S. Uchida, Phys. Rev. B **56**, 6295 (1997).

[7] K. Bender, K. Dietz, H. Enders, H. W. Hebberg, I. Hennig, H. J. Keller, H. W. Schaffer, and D. Schweitzer, Mol. Cryst. Liq. Cryst. **107**, 45 (1984).

[8] Y. Levi, O. Millo, A. Sharoni, Y. Tsabba, G. Leitas, and S. Reich, Europhys. Lett. **51**, 564 (2000).

[9] T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 438 (1982).

[10] (a) R. M. Pick, M. H. Cohen, and R. M. Martin, Phys. Rev. B **1**, 910 (1970); D. R. Penn, Phys. Rev. **128**, 2093 (1962); (b) M. Weger and J. L. Birman, cond-mat/0205279, Laser Phys. (to be published).

[11] A. Bianconi, N. L. Saini, A. Lanzara, M. Missori, T. Rosetti, H. Ohyanagi, H. Yamaguchi, K. Ota, and T. Ito, Phys. Rev. Lett. **76**, 3412 (1996); see also M. Weger, J. Supercond. **10**, 435 (1997).

[12] V. Heine, P. Nozières, and J. W. Wilkins, Philos. Mag. **13**, 741 (1966).

[13] J. L. Birman and M. Weger, Phys. Rev. B **64**, 174503 (2001).

[14] W. L. McMillan, Phys. Rev. **167**, 331 (1968).

[14a] M. Tinkham, *Introduction to Superconductivity*, 2nd ed. (McGraw-Hill, New York, 1996).

[15] H. Kamimura, K. Nomua, and A. Sano, J. Phys.: Condens. Matter **13**, 11435 (1998).

[16] P. W. Anderson, *Theory of Superconductivity of the High-$T_c$ Cuprates* (Princeton University Press, Princeton, NJ, 1997).

[17] D. Fay and M. Weger, Phys. Rev. B **62**, 15 208 (2000).

[17a] P. Monthoux, A. V. Balatsky, and D. Pines, Phys. Rev. B **46**, 14 803 (1992).

[18] E. Schachinger, J. P. Carbotte, and D. N. Basov, Europhys. Lett. **54**, 380 (2001).

[19] Z.-X. Shen, A. Lanzara, and N. Nagaosa, cond-mat/0102244 (unpublished); Nature (London) **412**, 510 (2001).

[20] S. H. Pan, J. P. O'Neal, R. L. Badzey, C. Chamon, H. Ding, J. R. Engelbrecht, Z. Wang, H. Eisaki, S. Uchida, A. K. Gupta, K. W. Ng, E. W. Hudson, K. M. Lang, and J. C. Davis, Nature (London) **403**, 282 (2001).

[21] R. E. Cohen, W. E. Pickett, H. Krakauer, and L. L. Boger, Physica B **150**, 61 (1988).

[22] Ralf Henn, Ph.D. thesis, Max Planck Institut, Stuttgart, 1997.

[23] J. Humlicek, A. P. Litvinchuk, W. Kress, B. Lederle, C. Thomsen, M. Cardona, H. U. Habermeier, E. Trafimov, and W. Konig, Physica C **206**, 345 (1993).

[24] M. Reedyk and T. Timusk, Phys. Rev. Lett. **69**, 2705 (1992).

[25] Z. Wang, J. R. Engelbrecht, S. Wang, H. Ding, and S. H. Pan, Phys. Rev. B **65**, 064509 (2002).

[26] J. C. Phillips and J. Jung, cond-mat/0103167 (unpublished), and references therein.