[30] Commercial supplier No. 1 (unpublished).

[31] Commercial supplier No. 2 (unpublished).

[32] C. M. Wolfe, G. E. Stillman, and J. O. Dimmock, J. Appl. Phys. 41, 504 (1970).

[33] R. Solomon, in Ref. 27, p. 11.

[34] O. V. Emelyanenko, D. N. Nasledov, V. G. Sidorov, V. A. Skripkin, and G. N. Talalakin, Phys. Status Solidi 12, K93 (1965).

PHYSICAL REVIEW B VOLUME 3, NUMBER 8 15 APRIL 1971

Dielectric Screening in a Layered Electron Gas

P. B. Visscher and L. M. Falicov
Department of Physics, University of California, Berkeley, California* 94720

(Received 13 October 1970)

A model anisotropic system, suggestive of the graphite structure, is investigated: It consists of a series of equally spaced parallel planes. A finite two-dimensional density of electrons in each plane is allowed to move freely in the plane, but tunneling between planes does not take place. The dielectric screening of a point charge is evaluated exactly in the random-phase approximation. For realistic electron densities and interlayer separations the screened potential drops off very rapidly both in the plane of the charge and perpendicular to it. The induced charge density is determined, and validity of the Thomas-Fermi approximation is discussed.

I. INTRODUCTION

In this paper we calculate the screening properties of a model anisotropic system, chosen for its resemblance to the graphite structure. The system consists of electrons constrained to move on parallel equally spaced planes; the single-particle states in the absence of interactions are two-dimensional plane waves.

The screening properties are investigated by calculating the dielectric response of the system to an external point charge on one of the planes. We use the self-consistent-field dielectric formulation of Ehrenreich and Cohen,[1] which is equivalent to the random-phase approximation (RPA). We introduce an infinitesimal perturbation V^{ext} (taken to be e^2/r), compute the induced potential V^{ind} owing to the density fluctuations caused by some total potential V^{tot}, and solve $V^{\text{tot}} = V^{\text{ext}} + V^{\text{ind}}$ for V^{tot}.

It is of interest to see whether there is a strong anisotropy in the screening, with the total potential decreasing at very different rates in the plane of the test charge and perpendicular to it. It is found that, in spite of the extreme anisotropy of the model, the screening lengths are comparable, and only under very extreme conditions is such strongly anisotropic screening found.

II. DERIVATION OF SELF-CONSISTENT-FIELD EQUATIONS

Consider a system of noninteracting electrons moving in a potential which depends only on z and has very narrow deep potential wells centered around $z = 0, \pm c, \pm 2c, \ldots$. For purposes of normalization assume $\vec{r} \equiv (x, y)$ is confined to a region of area A. The unperturbed eigenstates will then have wave functions

$$\psi_{\vec{k},\sigma,m}(\vec{r}, z) = A^{-1/2} a_\sigma e^{i\vec{k}\cdot\vec{r}} \chi(z - mc),$$

where $\vec{k}$ is a two-dimensional vector, the integer m labels the planes, and a_σ is a spin eigenfunction.

We consider only the limit in which the wells are arbitrarily deep and narrow, so that only the lowest one-dimensional eigenstate $\chi(z)$ can be occupied by an electron of finite energy. $\chi(z)$ is then effectively the square root of a δ function; that is, it is arbitrarily highly localized and

$$\int_{-\epsilon}^{\epsilon} \chi^2(z)\, dz = 1$$

for any $\epsilon > 0$.

Except for the energy contribution due to χ (which is the same for all states), the unperturbed eigenvalues are

$$E_{\vec{k},\sigma,m} = E_{\vec{k}} = (\hbar^2/2m_e)k^2 .$$

Assume the system is in its unperturbed (noninteracting) ground state, with a two-dimensional "Fermi disk" of radius k_F, where

$$An = \sum_{|\vec{k}| < k_F} 2 = \frac{2A}{(2\pi)^2}\, \pi k_F^2 .$$

Thus the density of electrons (per unit area) n is

$$n = k_F^2/2\pi .$$

The one-particle density matrix is then

$$\rho_0 = \sum_{\substack{|k| < k_F \\ \sigma, m}} |\vec{k}, \sigma, m\rangle\langle\vec{k}, \sigma, m| = \sum_s f_s\, |s\rangle\langle s| ,$$

where $s = (\vec{k}, \sigma, m)$ and f_s is the occupation number.

When we introduce the external potential V^{ext}, the density matrix becomes

$$\rho = \rho_0 + \rho' ,$$

and the first-order perturbation ρ' may be determined from the equation of motion[1] for ρ:

$$i\hbar\dot{\rho} = [\mathcal{H}, \rho].$$

Here the total Hamiltonian is $\mathcal{H} = \mathcal{H}_0 + V^{\text{tot}}$, where $\mathcal{H}_0$ is the unperturbed Hamiltonian and V^{tot} is the total perturbation. Thus to first order, the perturbed stationary state[2] is given by

$$0 = [\mathcal{H}_0, \rho'] + [V^{\text{tot}}, \rho_0],$$

or equivalently by

$$0 = (E_s - E_{s'})\rho'_{ss'} + (f_{s'} - f_s) V^{\text{tot}}_{ss'} ,$$
$$\rho'_{ss'} = \left(\frac{f_{s'} - f_s}{E_{s'} - E_s} \right) V^{\text{tot}}_{ss'} . \tag{2.1}$$

This changed density matrix gives rise to changes in the two-dimensional charge density $N_m(\vec{r})$ at position $\vec{r}$ on the mth plane, and thus induces a potential $V^{\text{ind}}_m(\vec{r})$. The self-consistency will be introduced by requiring that the V^{tot} in (2.1) be given by

$$V^{\text{tot}} = V^{\text{ext}} + V^{\text{ind}} . \tag{2.2}$$

Here V^{ext} is the potential of a point charge. It has matrix elements

$$V^{\text{ext}}_{ss'} = V^{\text{ext}}_{\vec{k}\sigma m, \vec{k}'\sigma' m'} = \delta_{\sigma\sigma'}\, \delta_{mm'}\, A^{-1} \times \int e^{i(\vec{k}' - \vec{k})\cdot\vec{r}} \frac{e^2 d^2\vec{r}}{(r^2 + m^2 c^2)^{1/2}} .$$

Thus the matrix element of V^{ext} is diagonal in the spin σ and the plane label m, and depends only on $q = |\vec{q}| = |\vec{k}' - \vec{k}|$ and on m. This will be true of the induced potential if it is true of the total potential so it is consistent to assume it for all of them. Thus we suppress the Kronecker δ's and all indices except m and q, and write for the matrix element

$$V^{\text{ext}}_{m,q} = A^{-1} (2\pi e^2/q) F_m(q) , \tag{2.3}$$

where

$$F_m(q) \equiv \frac{q}{2\pi} \int \frac{e^{i\vec{q}\cdot\vec{r}}}{(r^2 + m^2 c^2)^{1/2}}\, d^2\vec{r} \tag{2.4}$$

is a dimensionless integral, to be evaluated later.

The one-particle density operator (to be distinguished from the Dirac density matrix ρ) whose expectation value is the density at $\vec{R}$ is given in the coordinate representation by

$$[d(\vec{R})]_{\vec{R}_1;\vec{R}_2} = \delta(\vec{R} - \vec{R}_1)\, \delta(\vec{R} - \vec{R}_2) .$$

The two-dimensional density, of interest in our problem, is (on plane p)

$$N_p(\vec{r}) = \int_{pc-\epsilon}^{pc+\epsilon} dz\, [d(\vec{r}, z)]$$

whose coordinate representation is then

$$[N_p(\vec{r})]_{\vec{r}_1, z_1; \vec{r}_2, z_2} = \int_{pc-\epsilon}^{pc+\epsilon} dz\, \delta(\vec{r} - \vec{r}_1)\delta(z - z_1) \times \delta(\vec{r} - \vec{r}_2)\, \delta(z - z_2)$$
$$= \delta(\vec{r} - \vec{r}_1)\, \delta(\vec{r} - \vec{r}_2)\, \delta(z_1 - z_2) \quad \text{if } |z_2 - pc| < \epsilon .$$
$$= 0 \qquad \text{otherwise.}$$

The matrix element of $N_p(\vec{r})$ between $\psi_{k'\sigma' m'}$ and $\psi_{k\sigma m}$ thus vanishes if $m \neq m'$, $m \neq p$, or $\sigma \neq \sigma'$ and is otherwise

$$A^{-1} \int d^2 r_1\, dz_1 \int d^2 r_2\, dz_2\, e^{-i\vec{k}\cdot\vec{r}_1} e^{i\vec{k}'\cdot\vec{r}_2} \cdot \chi^*(z_1)\, \chi(z_2) \times \delta(\vec{r} - \vec{r}_1)\, \delta(\vec{r} - \vec{r}_2)\, \delta(z_1 - z_2) = A^{-1} e^{i(\vec{k}' - \vec{k})\cdot\vec{r}} . \tag{2.5}$$

To find the expectation value of the one-particle two-dimensional density operator we multiply by the Dirac density matrix ρ and take the trace. We find that the perturbation in the density is given by

$$n_p(\vec{r}) = \text{Tr}[\rho' N_p(\vec{r})] = \sum_{ss'} \rho'_{ss'} [N_p(\vec{r})]_{s's}$$
$$= A^{-1} \sum_{\sigma, k, k'} \frac{f_{k'} - f_k}{E_{k'} - E_k} V^{\text{tot}}_{p, k'-k}\, e^{i(\vec{k}' - \vec{k})\cdot\vec{r}} \tag{2.6}$$

[we have used (2.1) and (2.5) and noted that $V^{\text{tot}}_{ss'}$ depends only on $\vec{k}' - \vec{k} = \vec{q}$ and m],

$$n_p(\vec{r}) = \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}}\, n_{p,q} ,$$

where

$$n_{p,q} \equiv -\frac{q}{2\pi e^2} D(q)\, V^{\text{tot}}_{p,q} \tag{2.7}$$

and

$$D(q) \equiv -\frac{2\pi e^2}{qA} \sum_{\sigma, \vec{k}} \frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}}}{E_{\vec{k}+\vec{q}} - E_{\vec{k}}} \tag{2.8}$$

[the factor $q/2\pi e^2$ is inserted so $D(q)$ will be dimensionless]. This density perturbation induces a potential V^{ind}

$$V^{\text{ind}}_p(\vec{r}) = \sum_{p'} \int d^2\vec{r}' \frac{e^2}{[(\vec{r}' - \vec{r})^2 + c^2(p - p')^2]^{1/2}}\, n_{p'}(\vec{r})$$
$$= \sum_{p'} \sum_{\vec{q}} n_{p',q} \int d^2\vec{r}' \frac{e^2}{[(\vec{r}' - \vec{r})^2 + c^2(p - p')^2]^{1/2}}\, e^{i\vec{q}\cdot\vec{r}'}$$
$$= \sum_{p'} \sum_{\vec{q}} n_{p',q} \frac{2\pi e^2}{q} F_{p-p'}(q)\, e^{i\vec{q}\cdot\vec{r}}$$

[F is defined by (2.4)]. Since the matrix element of

$e^{i\vec{q}\cdot\vec{r}}$ between states $\vec{k}$ and $\vec{k}'$ is $\delta_{\vec{q},\vec{k}-\vec{k}'}$, we obtain for the matrix element of V_p^{ind}

$$V^{\text{ind}}_{p,-\vec{q}} = \sum_{p'} n_{p',q} \frac{2\pi e^2}{q} F_{p-p'}(q), \tag{2.9}$$

where we may replace $[-\vec{q}]$ by $\vec{q}$ because of the symmetry of the problem.

Using (2.3), (2.7), and (2.9) we may write the self-consistency equation (2.2) as

$$g_{m,q} = F_m(q) - D(q)\sum_p F_{m-p}(q) g_{p,q} , \tag{2.10}$$

where

$$g_{m,q} \equiv A(q/2\pi e^2)V^{\text{tot}}_{m,q} \tag{2.11}$$

is the dimensionless potential.

In Sec. III we evaluate the integrals (2.4) and (2.8), and solve exactly for the total potential g; in Sec. IV we Fourier transform it into real space and present some numerical calculations.

It is interesting first to see what form (2.10) takes in the Thomas-Fermi (TF) approximation. Instead of finding the induced density $n_p(\vec{r})$ by treating V^{tot} as a quantum-mechanical perturbation, we assume $n_p(\vec{r})$ is determined by a local Fermi level which changes with V^{tot} in such a way that the total energy of an electron at the Fermi level remains constant. Since in two dimensions the energy and the density are both proportional to k_F^2, they are proportional to each other. The deviation of the density from its unperturbed value is given by

$$n_m(\vec{r}) = (m_e/\hbar^2\pi)V^{\text{tot}}_m(\vec{r}) . \tag{2.12}$$

The screening length is related to the proportionality factor in (2.12); in three dimensions it depends on k_F and causes the screening to become less effective when k_F is small. The surprising consequence of (2.12) for the two-dimensional system is that the TF screening behavior is *independent* of k_F. Of course as k_F approaches zero there can be no screening, so the TF approximation breaks down very badly in this limit. But even for small electron concentrations, the actual screening, as given by RPA is fairly strong.

The TF screening may be calculated quantitatively by noting that if we use (2.12) in place of (2.7) to relate n to V^{tot}, the solution of the self-consistency equation (2.10) proceeds in the same way with $D(q)$ replaced by

$$D_{\text{TF}}(q) = -2/qa_0 , \tag{2.13}$$

where a_0 is the Bohr radius.

III. SOLUTION OF SELF-CONSISTENT-FIELD EQUATIONS

The quantity $D(q)$, defined in (2.8), can be written in integral form

$$D(q) = -\frac{e^2}{\pi q}\int d^2\vec{k}\,\frac{f_{\vec{k}+\vec{q}} - f_{\vec{k}}}{(\hbar^2/2m_e)[(\vec{k}+\vec{q})^2 - k^2]} .$$

This can be easily reduced to

$$D(q) = -(2/\pi q a_0)I(q/k_F),$$

where a_0 is an effective-mass Bohr radius

$$a_0 = \hbar^2/m_e e^2 ,$$

and

$$I(q/k_F) \equiv \int_{\substack{|\vec{k}|>k_F \\ |\vec{k}+\vec{q}|<k_F}} 2(2\vec{q}\cdot\vec{k} + q^2)^{-1} d^2\vec{k} .$$

If we set

$$B \equiv q/k_F , \quad u \equiv k_\perp/k_F , \quad v \equiv k_\parallel/k_F ,$$

($k_\perp$ and $k_\parallel$ are the components of $\vec{k}$ perpendicular and parallel to $\vec{q}$) the integral becomes

$$I(B) = \int_{-1}^{1} du \int_{-B-(1-u^2)^{1/2}}^{-B+(1-u^2)^{1/2}} dv\, 2(2Bv + B^2)^{-1} .$$

We have assumed $B > (1-u^2)^{1/2}$; otherwise the limits on v will be different, but we will obtain the same result

$$I(B) = \int_{-1}^{1} du \frac{1}{B}\log\left|\frac{2(1-u^2)^{1/2} - B}{-2(1-u^2)^{1/2} - B}\right| .$$

So far the calculation is very much like that leading to the Lindhard[3] dielectric function in three dimensions, where an extra factor of u in the integral makes it easy to evaluate. In the present case, however, the indefinite integral cannot be evaluated. The definite integral may be computed by contour integration; letting $u = \cos\theta$ and $z = e^{i\theta}$ it becomes the integral over the unit circle

$$I(B) = \frac{1}{2B}\,\text{Im}\int_{|z|=1} \frac{dz}{i}\log\left|\frac{z^2 - 1 + izB}{z^2 - 1 - izB}\right| . \tag{3.1}$$

It is necessary to treat this separately for $B < 2$ and $B > 2$. In the former case the cut in the log gives two cuts, along the left and right sides of the unit circle, respectively (the log of the absolute value must be regarded as the real part of the analytic log function). The integral of the logarithm is zero, since it is analytic within the circle; hence we may find the integral of the real part by integrating the imaginary part and multiplying by $-i$. The imaginary part being just π, we need only compute the differences between the ends of the cuts. We obtain the simple result π for the expression $I(B)$.

In the other case ($B > 2$) the cut in the log gives rise to a cut within the unit circle, along the imaginary axis. Thus the integral around the unit circle is just the integral around the cut, which is again trivial since the discontinuity across the cut is just $2\pi i$. This time the final result is $I(B)=\pi[1-(1-4/B^2)^{1/2}]$. Putting this into the expression for $D(q)$ gives

$$\begin{aligned} D(q) &= \frac{-2}{qa_0}\times\ 1 \qquad (q<2k_F) \\ &= \frac{-2}{qa_0}\times\ [1-(1-4k_F^2/q^2)^{1/2}] \quad (q>2k_F). \end{aligned} \tag{3. 2}$$

This is identical with the TF result (2. 13) for $q<2k_F$.

We will also need the quantity $F_m(q)$ defined in (2. 3),

$$F_m(q)=\frac{q}{2\pi}\int\frac{e^{i\vec{q}\cdot\vec{r}}}{(r^2+m^2c^2)^{1/2}}\,d^2\vec{r}\,,$$

giving the Fourier transform of the potential of an external point charge m planes away. By the Fourier inversion theorem it is equivalent to require

$$\frac{1}{(r^2+m^2c^2)^{1/2}}=\frac{1}{2\pi}\int e^{-i\vec{q}\cdot\vec{r}}\,\frac{F_m(q)}{q}\,d^2\vec{q}\,. \tag{3. 3}$$

Using the integral representation of the Bessel function of order zero

$$2\pi J_0(qr)=\int_0^{2\pi}e^{iqr\cos\theta}\,d\theta\,, \tag{3. 4}$$

we obtain

$$\frac{1}{(r^2+m^2c^2)^{1/2}}=\int_0^\infty J_0(qr)F_m(q)\,dq\,.$$

This equation is satisfied[4] by

$$F_m(q)=e^{-|qmc|}\,. \tag{3. 5}$$

Having evaluated all the functions appearing in the self-consistency equation (2. 10) for the potentials, we proceed to solve it. The different q vectors are completely uncoupled; however, the potentials on the various planes (labeled by m) remain coupled. They may be straightforwardly uncoupled by Fourier analyzing all terms with respect to m (the integer labeling the successive planes) and inverting the transform by a contour integral. As this is extremely laborious, and leads to the simple result that $g_{m,q}$ is a geometric series in m, we will content ourselves with assuming

$$g_m=ht^m\,, \tag{3. 6}$$

and solving for the constants h and t. (These depend on q, of course, as does g_m, but we will suppress the q subscript.) Since the $F_m(q)$ appearing in (2. 10) is also a geometric series in $|m|$,

$$F_m(q)=(e^{-qc})^{|m|}\equiv f^{\,|m|}\,, \tag{3. 7}$$

the equation may be broken into several geometric series (terminating where p or $m-p$ changes sign). When these are summed, the conditions that (2. 10) be satisfied for all m are

$$h=\frac{Dh}{1-t/f}-\frac{Dh}{1-tf}$$

and

$$0=1+\frac{Dh}{1-1/tf}-\frac{Dh}{1-t/f}\,,$$

which may easily be solved for h and t. The requirements of convergence of all the series ($|t|<1$, $|ft|<1$) rule out all but one solution. If we define

$$\begin{aligned} x &= f+f^{-1}+\frac{\sqrt{2}(f^{-1}-f)\rho_s}{B}\times\ 1 \qquad \text{if } B\leq 2 \\ &= f+f^{-1}+\frac{\sqrt{2}(f^{-1}-f)\rho_s}{B}\times[1-(1-4/B^2)^{1/2}] \\ &\qquad\qquad \text{if } B>2\,, \end{aligned} \tag{3. 8}$$

where f is defined in (3. 7), then

$$t=\tfrac{1}{2}[x-(x^2-4)^{1/2}] \tag{3. 9}$$

and

$$h=[t/(1-t^2)](f^{-1}-f). \tag{3. 10}$$

Thus for a given choice of k_F and c (interplane spacing) we may calculate the screened potential $g_{m,q}$ and numerically Fourier transform into real space.

IV. NUMERICAL RESULTS

The matrix elements

$$V^{\text{tot}}_{\vec{k}\sigma m,\vec{k}'\sigma' m'}=V^{\text{tot}}_{m,\vec{q}}$$

of the total potential depend only on $\vec{q}=\vec{k}'-\vec{k}$ and $m=m'$, so in real space the potential is

$$V_m^{\text{tot}}(\vec{r})=\sum_{\vec{q}}V^{\text{tot}}_{m,q}e^{-i\vec{q}\cdot\vec{r}}=\frac{A}{(2\pi)^2}\int d^2\vec{q}\,V^{\text{tot}}_{m,q}\,e^{-i\vec{q}\cdot\vec{r}}\,.$$

Using (2. 11) and (3. 4) we get

$$V_m^{\text{tot}}(\vec{r})=e^2\int_0^\infty g_{m,q}J_0(qr)\,dq\,, \tag{4. 1}$$

where $g_{m,q}$ is given by (3. 6). Similarly for the density we obtain from (2. 6) and (2. 7)

$$n_m(\vec{r})=\frac{-1}{2\pi}\int_0^\infty g_{m,q}D(q)J_0(qr)q\,dq\,. \tag{4. 2}$$

There are two input parameters which must be specified to evaluate the potential: the interplanar spacing c and the electron concentration n, which we shall convert to an average interparticle distance ρ_s such that $\pi\rho_s^2 n=1$ (analogous to the common r_s parameter in three dimensions[5]). Both c and ρ_s will be specified in units of the Bohr radius $a_0=\hbar^2/m_e e^2$, where m_e may be taken to be the effective mass of the two-dimensional band structure.[6]

In applying this model to graphite we must choose a reasonable electron concentration and effective mass. If we use the actual carrier concentration of $\sim 5.1\times10^{-5}$ electrons or holes per atom and the effective mass of about $m_e = 0.05m_0$,[7] we find dimensionless parameters $c = 0.32$ a.u. and $\rho_s = 25$ a.u. The potential calculated from (3.6), (3.8)–(3.10), and (4.1) for these parameters is very weakly screened. For $r \lesssim 2$ it is well given by $V(r) = e^2/r - 0.46$ a.u. Because it differs from the unscreened potential by a constant (this is also true if we move off the plane of the charge) the electric field is virtually unscreened. Because of our choice of the Bohr radius as the unit of length (it is in this case $a_0 = 10.6$ Å), $r = 2$ corresponds to 15 times the nearest-neighbor distance; the electric field at this distance is only 10% below its unscreened value. The potential passes through zero near $r = 3$, and reaches a minimum at about $r = 5$ (37 nearest-neighbor distances). The RPA is not a very good approximation for such a low-density gas,[5] but it is fairly clear that the short-range screening will not come out of a treatment which includes only the free carriers.[8] If we wish to analyze the short-range screening we must include more electrons than those which enter into the transport properties. We chose to take into account all of the π electrons; thus we used a set of parameters corresponding to a density of one electron per atom and a mass $m = m_0$, the bare electron mass; $c = 6.37$ a.u.; and $\rho_s = 1.729$ a.u. In this case, as in most cases of practical interest, the interplane spacing c somewhat exceeds ρ_s, the interparticle spacing in the plane. In this regime the screening is well described by a few approximate expressions [(4.4) and (4.5) below]. This condition $c \gtrsim \rho_s$ simplifies the problem because the potential of the first plane (RPA in Fig. 1) is not greatly affected by the other planes (letting $c \to \infty$ changes Fig. 1 only slightly). The TF approximation in Fig. 1 differs from the exact result in that it lacks the oscillations (Friedel[9] oscillations) of wavelength $2\pi/2k_F = 3.84$ a.u. These dominate the result at large distances, and are given [using (4.4) below] by

$$V_0^{\text{tot}}(r) \approx -(0.16/r^2)\sin(2k_F r) \text{ a.u.} \qquad (4.3)$$

As the electron concentration is increased (ρ_s decreased) the exact result approaches the TF potential in Fig. 1, as we expect from the fact that the TF approximation is a high-density limit. The TF result does not change with ρ_s (due to the anomalous nature of the two-dimensional gas discussed in Sec. III); for $\rho_s = 0.1729$ (one-tenth the graphite value) the exact potential is barely distinguishable from the TF potential of Fig. 1. This has a roughly exponential drop off; empirically

$$V_0^{\text{TF}}(r) \approx (0.082/r)\, e^{-0.45r} \text{ a.u.} \quad (r \gtrsim 2)\,. \qquad (4.4)$$

From (4.3) and (4.4) it is easily seen that $V_0(r)$ is dominated eventually by the Friedel oscillations, which drop off more slowly, though as ρ_s is decreased the value of r at which the oscillations take over increases. The amplitude of these oscillations (and hence the point where they dominate the TF behavior) may be obtained for arbitrary ρ_s, c, and m from (4.3) by a simple scaling argument based on the assumption that it is determined by the singularity in (3.1) at $B = 2$. Since the result is not very dependent on c for $c \gtrsim 1$, we give it only in the $c \to \infty$ limit (the fractional error is of order $e^{-4k_F c}$)

$$V_m^{\text{tot}} \approx -\tfrac{1}{2}(m+1)(1+k_F)^{-2}\left[e^{-2k_F c}/(1+k_F^{-1})\right]^m \times \sin(2k_F r)/r^2\,. \qquad (4.5)$$

Thus the screened potential (on plane $m = 0$) for an arbitrary density may be obtained by using the asymptotic form (4.5) for large r and adding in the TF result (4.4) when r is small enough for it to be significant. Very near the origin the TF result is always lower than the exact one [instead of approaching $(r^{-1} - \text{const})$ as does the exact potential, the TF result diverges as $(r^{-1} + A \log r)$], but the onset of the discrepancy approaches $r = 0$ as $\rho_s \to 0$.

The behavior of the potential at $r = 0$ on successive planes ($m = 1, 2, \ldots$) may also be estimated in the limit $c \to \infty$. The limiting forms of the formulas in Sec. III give

$$V_m^{\text{tot}}(r=0) \to (3S_m/2mc^2)(4c)^{-m}, \qquad (4.6)$$

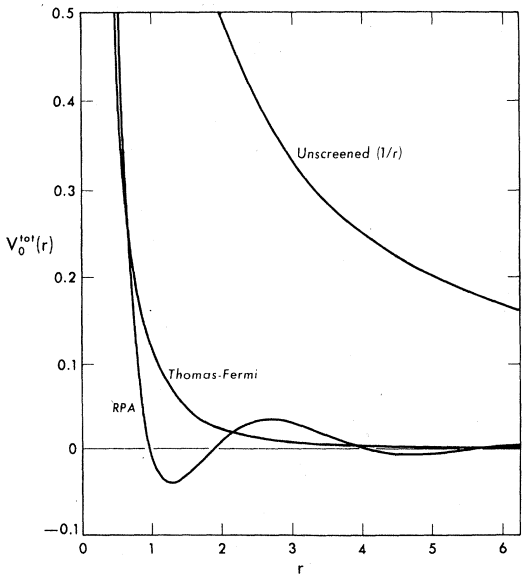

FIG. 1. Screened potential of a point charge on the plane $m = 0$ (parameters correspond to graphite). TF and unscreened results given for comparison.

where the integral

$$S_m = \tfrac{1}{3} m \int_0^{\infty} x^{m+1} (\sinh x)^{-m}\, dx$$

varies little with m. It can be evaluated[10] for $m = 1$:

$$S_1 = \tfrac{1}{3} \times \tfrac{7}{2}\, \zeta(3) = 1.40 \ ,$$

and the method of steepest descent gives

$$\lim_{m \to \infty} S_m = 1 \ .$$

In the case of the graphite parameters, the potential on the $m = 1$ plane is $V_1^{\text{tot}}(r = 0) = 1.37 \times 10^{-3}$ a.u. This is given fairly well by (4.6) which is 1.9×10^{-3} a.u. The $V_1^{\text{tot}}(r)$ is given extremely accurately for all r by the TF approximation. [It can be seen from (4.5) that the coefficient of the Friedel oscillations is about 10^{-5}.] The $m = 1$ potential would not be resolvable in Fig. 1.

Examination of (4.6) shows that the potential on the $m = 1$ plane is determined by the quadrupole field of the external charge with its diffuse ring of induced charge (the induced charge density is given in Fig. 2 for graphite). We see here another anomalous feature of the two-dimensional problem. The quadrupole moment of the induced charge distribution is independent of the electron concentration. Unlike the constant TF screening, the validity of this result is not restricted to the high-density limit. The quadrupole moment remains constant even at very low electron concentrations for which the screened potential bears no resemblance to the TF result of Fig. 1.

The potentials on the rest of the planes $m = 2$, 3, ... are seen also to have multipole behavior; the effect of each plane is to screen out the highest multipole, increasing the multipolarity by 1.

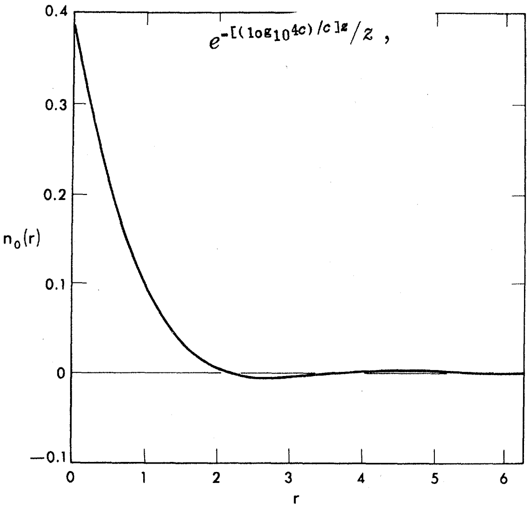

FIG. 2. Induced charge density producing the screening of Fig. 1.

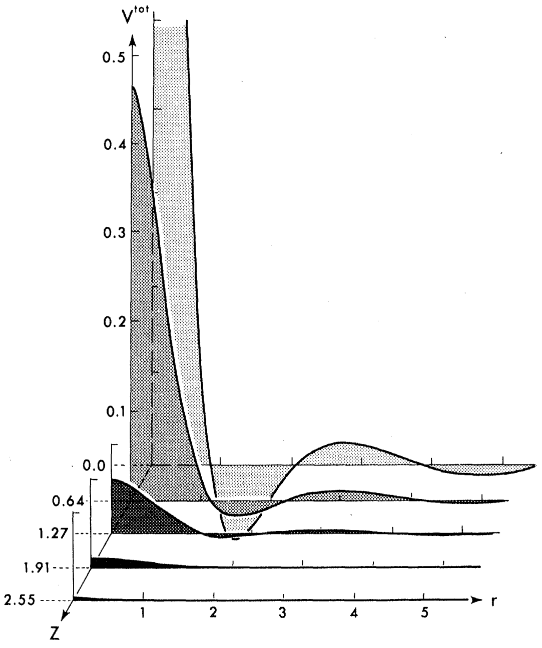

FIG. 3. Screened potential for the same number of electrons per unit area as graphite, but spacing $c = 0.637$ (layers packed ten times more densely than in graphite). Planes $m = 0, 1, 2, 3, 4$ are shown.

If we cast (4.6) into the standard exponential screening form, we find

$$V_m^{\text{tot}}(r = 0) = (3S_m/2c)\, e^{-[(\log 4c)/c]z}/z, \tag{4.7}$$

where $z = mc$. Thus we still get exponential screening, but with a screening distance that increases almost as the interplane spacing c.

It is interesting to compare several screening parameters for the case of graphite. Defining λ in each case so that $V(r) = \text{const} \times e^{-\lambda r/r}$, we find that for a three-dimensional gas with the same density, $\lambda \sim 1.00$ a.u. From (4.7) the screening perpendicular to the layers is described by $\lambda \sim 0.51$. Within the plane we would have $\lambda \sim 0.45$ from (4.4), but the Friedel oscillations prevent exponential screening far from the external charge. Thus we find no marked anisotropy in the screening; the screening rate is reduced by about a factor of 2 in all directions from the value for the three-dimensional gas, and the Friedel oscillations become much more important (dropping off as r^{-2} instead of r^{-3} as they do in three dimensions).

In the low-density limit ($\rho_s \gg 1$) the actual potential becomes higher than the TF one everywhere, the Friedel oscillations move farther out, and the potential near the origin approaches the unscreened value $1/r$ at the upper right of Fig. 1. The induced charge distribution spreads out as ρ_s increases.

(The distance at which the density drops to half its value at the origin is of the order of $\rho_s^{2/3}$.) Most of the induced charge, thus, is concentrated in a region much smaller than ρ_s about the origin. Beyond this there are alternating rings of positive and negative charge whose width is proportional to ρ_s (these are the Friedel oscillations). The total charge in each ring is negligible, but they must be considered in calculating the quadrupole moment. (The moment of the central region increases indefinitely as ρ_s is increased, and a large number of rings must be summed over to obtain the constant quadrupole result mentioned above).

So far we have considered only cases in which $c > \rho_s$, and our approximations have assumed $c \to \infty$. But to see the self-consistent effects of interactions between planes, we must consider a case in which the separation c is small enough so that the planes with $m > 0$ have a significant effect on the $m = 0$ plane (this is not the case in graphite). Figure 3 shows the potential on several of the planes for $c = 0.637$ (layers ten times more closely packed than in graphite) using $\rho_s = 1.729$, the same as in graphite. There is no qualitative change in the potential on the plane of the charge ($m = 0$), though the presence of the other planes cause the potential to be screened out more rapidly. But the potential on the $m = 1$ plane is no longer given by the quadrupole field of the $m = 0$ plane as in (4.6). Because of the increased density of planes, the screening in the z direction is now much more rapid [it is qualitatively still given by (4.7)].

In conclusion we would like to point out that the rather unusual screening properties of layered structures should give related effects (and hopefully observable ones) in the phonon spectrum, superconducting properties, conductivity, etc. Although we have chosen our parameters so as to fit the values of graphite, which is by far the simplest of the layered structures, nature provides a fairly large collection of such materials. For example, the transition-metal dichalcogenides[11] are one such family, and the distance between the transition-metal ions can be increased by the insertion of layers of organic molecules, such as pyridine.[12] These systems show extremely large anisotropy in the conductivities of the layers and perpendicular to them, and some of them are superconducting. Our simple model could therefore be meaningful for them.

---

*Work supported in part by the National Science Foundation under Grant No. GP 13 889.

[1] H. Ehrenreich and M. H. Cohen, Phys. Rev. 115, 786 (1959).

[2] This treatment may easily be generalized to time-varying perturbations. For the two-dimensional electron gas (i.e., only one plane) the dielectric function for all frequencies and wave numbers was obtained by F. Stern, Phys. Rev. Letters 18, 546 (1967). Generalizing (2.1) to a frequency $\omega \neq 0$ introduces a term $\hbar\omega$ into the denominator, which does not complicate the calculations in any essential way. The plasmon dispersion relation (which Stern obtained for the two-dimensional gas) could then be obtained for the layered gas, although we have not pursued this.

[3] J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. No. 28, 8 (1954).

[4] H. B. Dwight, *Tables of Integrals and Other Mathematical Data* (Macmillan, New York, 1957), Eq. 875.1.

[5] D. Pines, Solid State Phys. 1, 367 (1955).

[6] For the rest of this paper we use effective-mass atomic units: $m_e = 1$, $\hbar = 1$, $e = 1$. Energies are therefore given in hartrees (27.2eV) if m_e is the free-electron mass.

[7] J. W. McClure, IBM J. 8, 255 (1964); A. P. Cracknell, Advan. Phys. 18, 681 (1969).

[8] A calculation of the dielectric screening of a charged impurity by the free carriers was done by A. D. Boardman and D. G. Graham [J. Phys. C 2, 2320 (1969)] in calculating the impurity-limited resistivity.

[9] J. M. Ziman, *Principles of the Theory of Solids* (Cambridge U. P., Cambridge, England, 1964), p. 137.

[10] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1965), Eq. 3.523.1.

[11] J. D. Wilson and A. D. Yoffe, Advan. Phys. 18, 193 (1969).

[12] F. R. Gamble, F. J. DiSalvo, R. A. Klemm, and T. H. Geballe, Science 168, 568 (1970).