Dielectric Properties of the Wigner and Related Dipole Lattices*

AMITABHA BAGCHI
Department of Physics, University of California, San Diego, La Jolla, California 92037
(Received 20 September 1968)

The low-density or Wigner limiting case of the electron gas is studied for its response to a longitudinal electric field. The long-wavelength static dielectric constant is seen to be negative. Some curious features of the dielectric function are explained by comparison of the electron "solid" with the classical Lorentz lattice, of which the Wigner lattice is seen to be a limiting case.

I. INTRODUCTION

A. General

THE low-density state of the electron gas was first investigated by Wigner,[1,2] who pointed out that in the presence of a uniform compensating background of positive charge the electron gas, at sufficiently high dilution, would form a regular lattice. This is because as the density of the electron gas is reduced, the Coulomb interactions dominate the kinetic energy of the electrons so that a configuration of the lowest potential energy, i.e., a regular array of electrons, is the favored ground state. The compensating positive background is assumed to be held rigidly fixed.

We begin with a review of the theory of oscillation of a Coulomb lattice and its phonon spectrum. (By a Coulomb lattice we mean a lattice of charges interacting via Coulomb forces only.) In Sec. II we discuss the response of the Wigner lattice first to a space-and-time-varying perturbing charge distribution and then to a fixed point charge. We derive an explicit expression for the frequency- and wave-vector-dependent dielectric constant and discuss its properties. Section III is devoted to relating the Wigner Electron "solid" to the classical Lorentz model for an insulator. We show that the Wigner lattice is a limiting case of the Lorentz model and this helps to explain some of the puzzling features of the dielectric function of the former.

B. Review of Lattice Vibrations

The vibration spectrum of a Coulomb lattice has been studied by several authors in the harmonic approximation.[3,4] The theory has been adequately summarized in Pines.[5] For our purpose we consider a lattice of electrons immersed in a fixed uniform sea of positive charge. In its undisturbed state the ith electron is at $\mathbf{R}_i$. Let U_i^α denote the αth Cartesian component of a small displacement of the ith electron. If we let $\mathbf{R}_i'=\mathbf{R}_i+\mathbf{U}_i$, the Hamiltonian for the system is

$$H=\sum_i \frac{p_i^2}{2m}+\tfrac{1}{2}[\sum_{i\neq j} V(\mathbf{R}_i'-\mathbf{R}_j')-\sum_{i\neq j} V(\mathbf{R}_i-\mathbf{R}_j)], \quad (1.1)$$

where

$$V(\mathbf{R}_i-\mathbf{R}_j)=\frac{e^2}{|\mathbf{R}_i-\mathbf{R}_j|}=\sum_{\mathbf{k}} V_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}, \quad (1.2)$$

with[6]

$$V_{\mathbf{k}}=4\pi e^2/k^2. \quad (1.3)$$

We can write, in the harmonic approximation,

$$H=\sum_i \frac{p_i^2}{2m}+\tfrac{1}{2}\sum_{i,j,\alpha,\beta} U_i^\alpha A_{ij}^{\alpha\beta} U_j^\beta. \quad (1.4)$$

Here

$$A_{ij}^{\alpha\beta}=\sum_{\mathbf{k}} k^\alpha k^\beta V_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}. \quad (1.5)$$

$$A_{ij}^{\alpha\beta}=-\sum_{\mathbf{k}}\sum_{j\neq i} k^\alpha k^\beta V_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}. \quad (1.6)$$

Equation (1.4) leads to the equations of motion

$$m\ddot{U}_i^\alpha(t)+\sum_{j,\beta} A_{ij}^{\alpha\beta} U_j^\beta(t)=0. \quad (1.7)$$

Exploiting translational invariance we look for solutions of the form

$$U_i^\alpha(t)=a(\mathbf{k},\lambda)\epsilon_{\mathbf{k}\lambda}^\alpha e^{i(\mathbf{k}\cdot\mathbf{R}_i-\omega(\mathbf{k},\lambda)t)}. \quad (1.8)$$

Here $\hat{\epsilon}_{\mathbf{k}\lambda}$ is an eigenvector belonging to $\mathbf{k}$ and the mode λ; $a(\mathbf{k},\lambda)$ is an amplitude factor. Substituting (1.8) in (1.7) we obtain, after a little manipulation

$$m\omega^2(\mathbf{k},\lambda)\epsilon_{\mathbf{k}\lambda}^\alpha=\sum_\beta\{\sum_j A_{ij}^{\alpha\beta} e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\}\epsilon_{\mathbf{k}\lambda}^\beta. \quad (1.9)$$

If the $A_{ij}^{\alpha\beta}$ are written out explicitly in terms of $V_{\mathbf{k}}$ by using (1.5) and (1.6) we obtain (cf. Ref. 5)

$$m\omega^2(\mathbf{k},\lambda)\hat{\epsilon}_{\mathbf{k}\lambda}=NV_{\mathbf{k}}\mathbf{k}(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda}) +N\sum_{\nu\neq 0}\{V_{\mathbf{k}+\mathbf{K}_\nu}(\mathbf{k}+\mathbf{K}_\nu)[(\mathbf{k}+\mathbf{K}_\nu)\cdot\hat{\epsilon}_{\mathbf{k}\lambda}] -V_{\mathbf{K}_\nu}\mathbf{K}_\nu(\mathbf{K}_\nu\cdot\hat{\epsilon}_{\mathbf{k}\lambda})\}. \quad (1.10)$$

K_ν here refer to the reciprocal lattice vectors. N is the number of electrons per unit volume. Use has been

* Work supported in part by the Office of Naval Research and the National Science Foundation.

[1] E. P. Wigner, Phys. Rev. **46**, 1002 (1934).
[2] E. P. Wigner, Trans. Faraday Soc. **34**, 678 (1938).
[3] C. B. Clark, Phys. Rev. **109**, 1133 (1958).
[4] R. A. Coldwell-Horsfall and A. A. Maradudin, J. Math. Phys. **1**, 395 (1960).
[5] D. Pines, *Elementary Excitations in Solids* (W. A. Benjamin, Inc., New York, 1963), Chap. 2.

[6] We choose normalization so that the total volume of our system, $\Omega=1$.

made in the derivation of (1.10) of the fact that, because of the compensating background, $V_{k=0}=0$. Finally, it follows from (1.9) that $\omega^2(\mathbf{k},\lambda)$ is an eigenvalue of a 3×3 matrix, for a given $\mathbf{k}$. The different eigenmodes for a given $\mathbf{k}$ are distinguished by the label λ which takes on the values 1, 2, and 3.

From Eq. (1.10) one derives the well-known sum rule[7]

$$\sum_{\lambda=1}^{3}\omega^2(\mathbf{k},\lambda)=\frac{4\pi Ne^2}{m}=\omega_p^2; \tag{1.11}$$

ω_p here is the electronic plasma frequency

In the long-wavelength limit ($k\to0$) one can talk of one strictly longitudinal mode for which $\hat{\epsilon}_{\mathbf{k}\lambda}\|\hat{k}$ and two transverse modes for which $\hat{\epsilon}_{\mathbf{k}\lambda}\perp\hat{k}$. Labeling the modes by l and t one can show from (1.10) that

$$\omega^2(\mathbf{k},l)\underset{\mathbf{k}\to0}{\longrightarrow}\omega_p^2;\quad \omega^2(\mathbf{k},t)\underset{\mathbf{k}\to0}{\longrightarrow}0. \tag{1.12}$$

For small but finite k, the two transverse frequencies are proportional to k. Using (1.11) the longitudinal frequency then takes the form

$$\omega^2(\mathbf{k},l)=\omega_p^2-a^2k^2. \tag{1.13}$$

Stability of the lattice demands that a^2 be positive. We note that for a finite $\mathbf{k}$ in a general direction the longitudinal mode does not necessarily lie in the direction of the wave vector.

II. DIELECTRIC PROPERTY

A. Response to a Longitudinal Electric Field

A knowledge of the frequency spectrum of the electron lattice enables one to discuss the frequency- and wave-vector-dependent longitudinal dielectric constant of the Wigner crystal. We imagine perturbing our system by introducing a charge distribution of the form

$$\rho_{\text{ext}}(\mathbf{r},t)=\rho_0e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}. \tag{2.1}$$

In this expression $\mathbf{k}$ is not restricted to the first Brillonin zone. From Poisson's equation the associated potential $\Phi_{\text{ext}}(\mathbf{r},t)$ and electric field $\mathbf{E}_{\text{ext}}(\mathbf{r},t)$ are

$$\Phi_{\text{ext}}(\mathbf{r},t)=(4\pi/k^2)\rho_0e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)},$$
$$\mathbf{E}_{\text{ext}}(\mathbf{r},t)=-\nabla\Phi_{\text{ext}}(\mathbf{r},t)=-i(4\pi\mathbf{k}/k^2)\rho_0e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}.$$

Evidently the driving force on the ith electron of charge $-e(e>0)$ is

$$\mathbf{F}_i(t)=-e\mathbf{E}_{\text{ext}}(\mathbf{R}_i,t)=i(4\pi\mathbf{k}/k^2)e\rho_0e^{i(\mathbf{k}\cdot\mathbf{R}_i-\omega t)}. \tag{2.2}$$

Denoting by $\mathbf{U}_i(t)$ the displacement of the ith electron we have the equation of motion

$$m\ddot{U}_i^{\alpha}(t)+\sum_{j,\beta}A_{ij}^{\alpha\beta}U_j^{\beta}(t)=F_i^{\alpha}(t). \tag{2.3}$$

[7] This was first derived by W. Kohn and D. Schechter (unpublished) quoted, e.g., in J. Bardeen and D. Pines, Phys. Rev. 99, 1140 (1955).

We write

$$U_i^{\alpha}(t)=\sum_{\lambda}a(\mathbf{k},\lambda)\epsilon_{\mathbf{k}\lambda}{}^{\alpha}e^{i(\mathbf{k}\cdot\mathbf{R}_i-\omega t)}. \tag{2.4}$$

Substituting this into the equation of motion (2.3) and using the fact that different phonon modes are independent we find

$$a(\mathbf{k},\lambda)=ie\rho_0\frac{4\pi}{k^2}\frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})}{m\{\omega^2(\mathbf{k},\lambda)-\omega^2\}}. \tag{2.5}$$

We may therefore write

$$\mathbf{U}_i(t)=\mathbf{U}^0e^{i(\mathbf{k}\cdot\mathbf{R}_i-\omega t)}, \tag{2.6}$$

where

$$\mathbf{U}^0=ie\rho_0\frac{4\pi}{k^2}\sum_{\lambda}\frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})\hat{\epsilon}_{\mathbf{k}\lambda}}{m\{\omega^2(\mathbf{k},\lambda)-\omega^2\}}, \tag{2.7}$$

and $\mathbf{U}$ is independent of $\mathbf{R}_i$.

In the original configuration the electron charge density of the system is

$$\rho(\mathbf{r})=-e\sum_i\delta(\mathbf{r}-\mathbf{R}_i)$$
$$=-e\sum_i\sum_{\mathbf{k}'}e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{R}_i)}. \tag{2.8}$$

After the introduction of the perturbing charge distribution the new charge density is

$$\rho_p(\mathbf{r},t)=-e\sum_i\sum_{\mathbf{k}'}e^{i\mathbf{k}'\cdot(\mathbf{r}-\mathbf{R}_i-\mathbf{U}_i)}. \tag{2.9}$$

The change in charge density to first order in $\mathbf{U}$ is clearly

$$\delta\rho(\mathbf{r},t)=\rho_p(\mathbf{r},t)-\rho(\mathbf{r})$$
$$=ieN\sum_{\nu}[(\mathbf{k}+\mathbf{K}_\nu)\cdot\mathbf{U}^0]e^{i[(\mathbf{k}+\mathbf{K}_\nu)\cdot\mathbf{r}-\omega t]}. \tag{2.10}$$

We find that the charge induced in the electron lattice by a perturbing charge of wave vector $\mathbf{k}$ involves all wave vectors $(\mathbf{k}+\mathbf{K}_\nu)$. For the space-averaged or "macroscopic" change in the charge density we select out of the sum in Eq. (2.10) only the term with $\mathbf{K}_\nu=0$. Labeling this part of $\delta\rho(\mathbf{r},t)$ by $\delta\rho^0(\mathbf{r},t)$ we have

$$\delta\rho^0(\mathbf{r},t)=ieN(\mathbf{k}\cdot\mathbf{U}^0)e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$$
$$=-\rho_0\frac{\omega_p^2}{k^2}\sum_{\lambda}\frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})^2}{[\omega^2(\mathbf{k},\lambda)-\omega^2]}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}. \tag{2.11}$$

The total space-averaged charge density at a point is

$$\rho_{\text{tot}}(\mathbf{r},t)=\rho_{\text{ext}}(\mathbf{r},t)+\delta\rho^0(\mathbf{r},t)$$
$$=\rho_0\left\{1-\frac{\omega_p^2}{k^2}\sum_{\lambda}\frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})^2}{[\omega^2(\mathbf{k},\lambda)-\omega^2]}\right\}e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}. \tag{2.12}$$

Now the longitudinal dielectric constant $\epsilon(\mathbf{k},\omega)$ is defined through

$$\rho_{\text{tot}}(\mathbf{r},t)=[\epsilon(\mathbf{k},\omega)]^{-1}\rho_{\text{ext}}(\mathbf{r},t). \tag{2.13}$$

Comparing (2.12) with (2.13) we arrive at the expression

$$\frac{1}{\epsilon(\mathbf{k},\omega)}=1-\frac{\omega_p^2}{k^2}\sum_\lambda \frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})^2}{[\omega^2(\mathbf{k},\lambda)-\omega^2]}. \tag{2.14}$$

We now consider a few limiting cases.

Case I: Arbitrary $\mathbf{k}$*; High Frequency* ($\omega\gg\omega_p$)

$$\frac{1}{\epsilon(\mathbf{k},\omega)}\approx 1+\frac{\omega_p^2}{k^2}\omega^{-2}\sum_\lambda (\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})^2$$

$$=1+\omega_p^2/\omega^2;$$

so

$$\epsilon(\mathbf{k},\omega)\approx 1-\omega_p^2/\omega^2. \tag{2.15}$$

This is an expected result, showing that at high frequency the lattice behaves like an electron plasma

Case II: Long Wavelength ($k\approx 0$)*; Arbitrary Frequency* ω

As $k\to 0$ the longitudinal mode points along $\mathbf{k}$ and its frequency approaches the plasma frequency. The transverse modes are normal to $\mathbf{k}$. It follows from (2.14) that in this limit

$$\epsilon(0,\omega)=1-\omega_p^2/\omega^2. \tag{2.16}$$

A plot of $\epsilon(0,\omega)$ against ω is shown in Fig. 1.

Case III: Static Response ($\omega=0$)

If in Eq. (2.14) we set $\omega=0$, then it readily follows that

$$\frac{1}{\epsilon(\mathbf{k},0)}=1-\frac{\omega_p^2}{k^2}\sum_\lambda \frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})^2}{\omega^2(\mathbf{k},\lambda)}. \tag{2.17}$$

But the sum rule of Eq. (1.11) shows that, for the lattice to be stable, we need

$$\omega^2(\mathbf{k},\lambda)\leq\omega_p^2 \quad (\lambda=1,2,3). \tag{2.18}$$

Combining Eqs. (2.17) and (2.18) we find that

$$\frac{1}{\epsilon(\mathbf{k},0)}\leq 1-\frac{\omega_p^2}{k^2}\sum_\lambda \frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})^2}{\omega_p^2},$$

which implies that, for all $\mathbf{k}$,

$$\epsilon(\mathbf{k},0)\leq 0. \tag{2.19}$$

The sign of the static dielectric constant of the electron lattice is surprising, especially when one remembers the result for the electron gas in the high density limit.

If $\mathbf{k}$ lies along a symmetric crystallographic direction and is small in magnitude it follows from Eq. (2.14) that

$$1/\epsilon(\mathbf{k},0)=1-\omega_p^2/\omega^2(\mathbf{k},l), \tag{2.20}$$

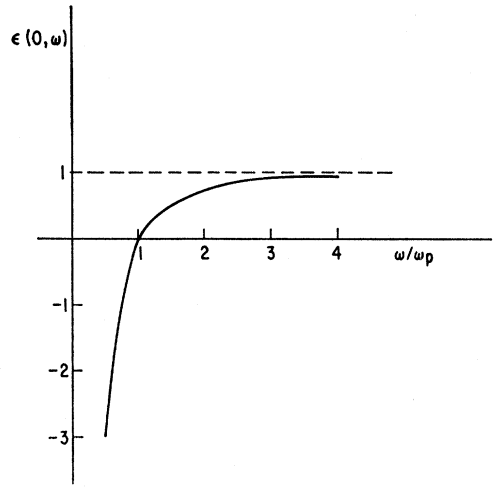

FIG. 1. The long-wavelength ($k=0$) dielectric constant of the Wigner lattice as a function of frequency.

where $\omega(k,l)$ is the longitudinal phonon frequency at wave vector $\mathbf{k}$. Using Eq. (1.13) in (2.20) we obtain

$$\epsilon(\mathbf{k},0)\xrightarrow[(ak)^2\ll\omega_p^2]{}1-\omega_p^2/a^2k^2. \tag{2.21}$$

A plot of $\epsilon(\mathbf{k},0)$ against k for small k is shown in Fig. 2.

From the preceding discussion we note that if we let $\omega\to 0$ and $k\to 0$, then independent of whether $k/\omega\to 0$ or $\omega/k\to 0$ we always have

$$\epsilon(0,0)=-\infty. \tag{2.22}$$

This result has been quoted in the literature.[8]

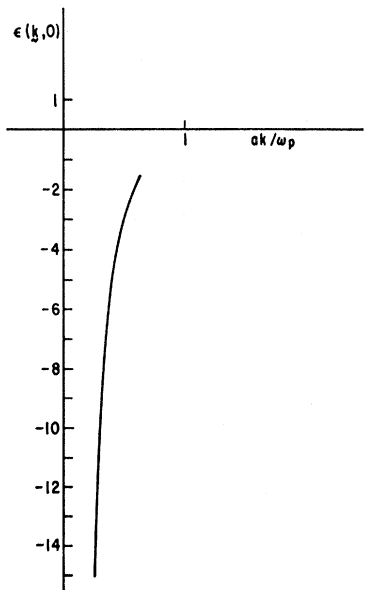

FIG. 2. The static-dielectric constant of the Wigner lattice as a function of wave vector k along a "good" crystallographic direction

[8] F. W. de Wette, Phys. Rev. 135, A287 (1964).

The negativity of the static dielectric constant of the Wigner crystal does not necessarily imply a lattice instability. The complete interaction between two electrons in the Wigner lattice involves not just the scalar dielectric constant defined in (2.17) but rather a dielectric tensor $\epsilon(\mathbf{k}+\mathbf{K}_\nu;\mathbf{k}+\mathbf{K}_{\nu'})$ as defined, for example, in Adler.[9] (Here $\mathbf{k}$ lies within the first Brillonin zone.) In (2.14) or (2.17) we have merely selected out for special consideration the diagonal element of the dielectric tensor with $\mathbf{K}_\nu=\mathbf{K}_{\nu'}$. The sign of such individual element is no indication of the stability of the entire lattice.

We note that the only possible lattice instability in our problem is phonon instability. This arises if there exists a phonon mode with an imaginary frequency. We investigated this possibility by adopting an interpolation scheme. Based on Clark's data,[3] for the phonon frequencies of a bcc Coulomb lattice in certain preferred crystallographic directions, we derived an interpolation formula for transverse phonon frequencies, for small $\mathbf{k}$ in a general direction, with the help of Kubic Harmonics. No imaginary phonon frequency was found in any direction so that we feel quite certain that the bcc Wigner lattice is stable.

We may, in fact, note that because of the stability of the lattice, coupled with the sum rule (1.11), we found in Eq. (1.13) that the longitudinal phonon frequency decreases with k (in the neighborhood of $k=0$) and this decrease is responsible for the negative dielectric constant.

B. Screening of a Static Point Charge

Consider a small point charge q placed at $\mathbf{r}$. The perturbing charge density is

$$\rho_{\text{ext}}(\mathbf{x})=q\delta(\mathbf{x}-\mathbf{r})=q\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{r})}. \tag{2.23}$$

The potential at $\mathbf{r}$ due solely to the perturbing charge is

$$\Phi_{\text{ext}}(\mathbf{x})=\frac{q}{|\mathbf{x}-\mathbf{r}|}=q\sum_{\mathbf{k}}\frac{4\pi}{k^2}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{r})}. \tag{2.24}$$

The electric field at the ith lattice point is

$$\mathbf{E}_{\text{ext}}(\mathbf{R}_i)=-\nabla\Phi_{\text{ext}}(\mathbf{x})|_{\mathbf{x}=\mathbf{R}_i}=-4\pi iq\sum_{\mathbf{k}}\frac{1}{k^2}\mathbf{k}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{r})}. \tag{2.25}$$

Therefore, the external force on the ith electron is

$$\mathbf{F}_i=-e\mathbf{E}_{\text{ext}}(\mathbf{R}_i)=ieq\sum_{\mathbf{k}}\frac{4\pi}{k^2}\mathbf{k}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{r})}. \tag{2.26}$$

[9] Stephen L. Adler, Phys. Rev. 126, 413 (1962).

The displacement of the ith electron, $\mathbf{U}_i$, can be expanded as

$$\mathbf{U}_i=\sum_{\mathbf{k},\lambda}a(\mathbf{k},\lambda)\hat{\epsilon}_{\mathbf{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{R}_i}. \tag{2.27}$$

In equilibrium we have the condition

$$\sum_{j,\beta}A_{ij}{}^{\alpha\beta}U_j{}^{\beta}=F_i{}^{\alpha}. \tag{2.28}$$

We substitute (2.27) into (2.28) and use the orthonormality property of $\hat{\epsilon}_{\mathbf{k}\lambda}$ to find

$$a(\mathbf{k},\lambda)=ieq\frac{4\pi}{k^2}\cdot\frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})}{m\omega^2(\mathbf{k},\lambda)}e^{-i\mathbf{k}\cdot\mathbf{r}}. \tag{2.29}$$

Consequently,

$$\mathbf{U}_i=ieq\sum_{\mathbf{k},\lambda}\frac{4\pi}{k^2}\frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})\hat{\epsilon}_{\mathbf{k}\lambda}}{m\omega^2(\mathbf{k},\lambda)}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{r})}. \tag{2.30}$$

We next turn to the problem of calculating the total electrostatic potential at the point $\mathbf{r}'$. The net potential at $\mathbf{r}'$ is

$$\begin{aligned}\Phi(\mathbf{r}')&=\frac{q}{|\mathbf{r}-\mathbf{r}'|}-e\sum_i\left\{\frac{1}{|\mathbf{R}_i+\mathbf{U}_i-\mathbf{r}'|}-\frac{1}{|\mathbf{R}_i-\mathbf{r}'|}\right\}\\&=q\sum_{\mathbf{k}}\frac{4\pi}{k^2}e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}-4\pi Ne^2q\sum_{\mathbf{k},\lambda}\sum_{\mathbf{K}_\nu}\frac{4\pi}{|\mathbf{k}+\mathbf{K}_\nu|^2}\frac{1}{k^2}\\&\quad\times\frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})[(\mathbf{k}+\mathbf{K}_\nu)\cdot\hat{\epsilon}_{\mathbf{k}\lambda}]}{m\omega^2(\mathbf{k},\lambda)}e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}e^{i\mathbf{K}_\nu\cdot\mathbf{r}'}.\end{aligned} \tag{2.31}$$

For a given vector separation $\mathbf{r}-\mathbf{r}'$ between the point charge and the point of observation, (2.31) depends on $\mathbf{K}_\nu\cdot\mathbf{r}'$, i.e., on the position of the point of observation relative to the lattice. If we keep $\mathbf{r}-\mathbf{r}'$ fixed but move $\mathbf{r}'$ (and consequently $\mathbf{r}$) over the entire crystal so as to average over it

$$\langle e^{i\mathbf{K}_\nu\cdot\mathbf{r}'}\rangle_{\text{av}}=0 \quad \text{if} \quad \mathbf{K}_\nu\neq 0. \tag{2.32}$$

Thus

$$\begin{aligned}\langle\Phi(\mathbf{r}')\rangle_{\text{av}}&=q\sum_{\mathbf{k}}\frac{4\pi}{k^2}\left[1-\frac{\omega_p{}^2}{k^2}\sum_{\lambda}\frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})^2}{\omega^2(\mathbf{k},\lambda)}\right]e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\\&=q\sum_{\mathbf{k}}\frac{4\pi}{k^2}\frac{1}{\epsilon(\mathbf{k},0)}e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}.\end{aligned} \tag{2.33}$$

The function $\epsilon(\mathbf{k},0)$ is given in Eq. (2.17). For small values of k it behaves as $-\omega_p{}^2/a^2k^2$ [see Eq. (2.21)] which is negative and removes the k^{-2} singularity of the unscreened Coulomb potential. Furthermore, $\epsilon^{-1}(\mathbf{k},0)$ has singularities at reciprocal lattice vectors [due to the vanishing of the transverse $\omega^2(\mathbf{k},\lambda)$ at such points] which will influence the asymptotic behavior of $\langle\Phi(\mathbf{r}')\rangle_{\text{av}}$. A detailed study of the asymptotic behavior did not seem worthwhile to us; but it is quite clear that it is totally different from the simple,

reduced Coulomb-like field produced by a point charge in a conventional dielectric.

III. WIGNER LATTICE AS LIMITING CASE OF THE LORENTZ MODEL

The Lorentz model for an insulator consists of a lattice of point charges $(-e)$ bound harmonically to their equilibrium positions by a restoring force characterized by the frequency ω_0. Let m be the mass of each point charge and N the number of lattice points per unit volume. Because of the requirement of charge neutrality a stationary charge $(+e)$ must be imagined as residing at each lattice point. The displacement of any negative charge, therefore, gives rise to a dipole, and thus we encounter a conventional dipole lattice. The static electric polarizability of each atom is

$$\alpha(\omega=0)=e^2/m\omega_0^2. \tag{3.1}$$

Consider a general configuration of the system with the ith charge suffering a displacement $\mathbf{U}_i$ so that the ith dipole has a moment $\mathbf{p}_i=-e\mathbf{U}_i$. The change in potential energy from the equilibrium configuration, in which all $\mathbf{U}_i$'s vanish, is easily seen to be

$$\Delta V_L=\tfrac{1}{2}m\omega_0^2\sum_{i,\alpha}U_i^\alpha U_i^\alpha + \tfrac{1}{2}\sum_{i,j,\alpha,\beta}{}'\left[\frac{p_i^\alpha p_j^\beta|\mathbf{R}_{ij}|^2\delta_{\alpha\beta}-3(p_i^\alpha R_{ij}^\alpha)(p_j^\beta R_{ij}^\beta)}{|\mathbf{R}_{ij}|^5}\right], \tag{3.2}$$

where

$$\mathbf{R}_{ij}\equiv\mathbf{R}_i-\mathbf{R}_j$$

and the prime in summation denotes exclusion of terms with $i=j$. Equation (3.2) may be rewritten as

$$\Delta V_L=\tfrac{1}{2}m\omega_0^2\sum_{i,\alpha}U_i^\alpha U_i^\alpha+\tfrac{1}{2}\sum_{i,j,\alpha,\beta}{}'A_{ij}^{\alpha\beta}U_i^\alpha U_j^\beta, \tag{3.3}$$

where

$$A_{ij}^{\alpha\beta}(i\neq j)=e^2\left[\frac{\delta_{\alpha\beta}|\mathbf{R}_{ij}|^2-3R_{ij}^\alpha R_{ij}^\beta}{|\mathbf{R}_{ij}|^5}\right], \tag{3.4}$$

and it is identical with $A_{ij}^{\alpha\beta}$ defined in (1.5).

Under the same electronic displacement the change in energy of the Wigner crystal may be written as [cf. Eq. (1.4)]

$$\Delta V_W=\tfrac{1}{2}\sum_{i,\alpha,\beta}A_{ii}^{\alpha\beta}U_i^\alpha U_i^\beta+\tfrac{1}{2}\sum_{i,j,\alpha,\beta}{}'A_{ij}^{\alpha\beta}U_i^\alpha U_j^\beta. \tag{3.5}$$

Since

$$A_{ii}^{\alpha\beta}=\delta_{\alpha\beta}m\omega_p^2/3, \tag{3.6}$$

as can be easily shown by using Poisson's equation and arguments of cubic symmetry, it follows that

$$\Delta V_W=\tfrac{1}{2}\sum_{i,\alpha}\tfrac{1}{3}m\omega_p^2U_i^\alpha U_i^\alpha+\tfrac{1}{2}\sum_{i,j,\alpha,\beta}{}'A_{ij}^{\alpha\beta}U_i^\alpha U_j^\beta. \tag{3.7}$$

Comparison with Eq. (3.3) indicates that the Wigner lattice is a special, limiting case of the Lorentz model with $\omega_0=\omega_p/\sqrt{3}$. The reason for calling it a limiting case will be discussed later. Of course, this assumes that the moving charge in the Lorentz model is a single electron, so that the mass m appearing in Eq. (3.1) is the electronic mass.

Using (3.7) one may rewrite (3.3) as

$$\Delta V_L=\Delta V_W+\tfrac{1}{2}m(\omega_0^2-\omega_p^2/3)\sum_{i,\alpha}U_i^\alpha U_i^\alpha. \tag{3.8}$$

To find the phonon frequencies in the Lorentz model one has to diagonalize a potential matrix which differs from the potential matrix for the Wigner crystal only in the diagonal elements, the difference being just a constant. If $\Omega(\mathbf{k},\lambda)$ denotes the phonon frequency in the Lorentz model for wave vector $\mathbf{k}$ and polarization λ then in terms of $\omega(\mathbf{k},\lambda)$, the Wigner lattice phonon frequency, we have

$$\Omega^2(\mathbf{k},\lambda)=\omega^2(\mathbf{k},\lambda)+\omega_1^2, \tag{3.9}$$

where we have defined

$$\omega_1^2=\omega_0^2-\omega_p^2/3. \tag{3.10}$$

We see immediately from (3.9) and (3.10) that if $\omega_0^2<\omega_p^2/\sqrt{3}$, i.e. if the Lorentz lattice has weaker restoring force than the Wigner lattice, the long-wavelength transverse phonon frequencies become imaginary and the lattice is unstable. Thus, the Wigner lattice can be regarded as a Lorentz lattice just on the verge of instability. In other words, if the natural frequency ω_0 of a stable Lorentz lattice is slowly reduced, then the limit when the lattice is just barely stable, we get the Wigner crystal. From here on we shall discuss a stable Lorentz lattice in which ω_1^2 of (3.10) is a small positive quantity.

The dielectric response of the Lorentz model can be worked out in the same way as in Sec. II for the Wigner crystal. In particular, the frequency- and wave-vector-dependent dielectric constant is given by

$$\frac{1}{\epsilon_L(\mathbf{k},\omega)}=1-\frac{\omega_p^2}{k^2}\sum_\lambda\frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})^2}{[\Omega^2(\mathbf{k},\lambda)-\omega^2]} =1-\frac{\omega_p^2}{k^2}\sum_\lambda\frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})^2}{[\omega^2(\mathbf{k},\lambda)+\omega_1^2-\omega^2]}. \tag{3.11}$$

A few limiting cases of this expression are discussed below.

Case I: Long-Wavelength ($k=0$); Arbitrary Frequency, ω

As $k\to 0$,

$$\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda}=k \text{ for the longitudinal mode;}$$
$$=0 \text{ for the transverse modes.}$$

And

$$\omega^2(\mathbf{k},l)=\omega_p^2.$$

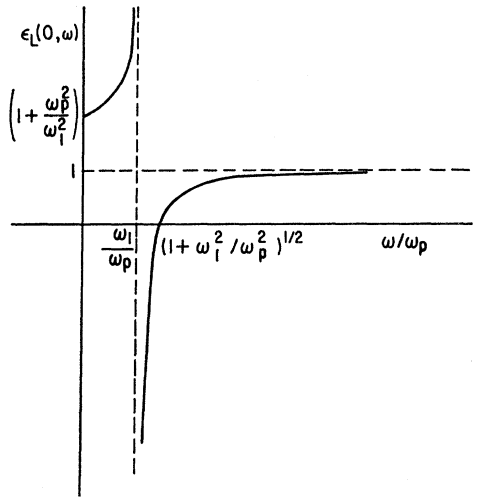

FIG. 3. The dielectric constant of the Lorentz lattice in the long-wavelength limit as a function of frequency.

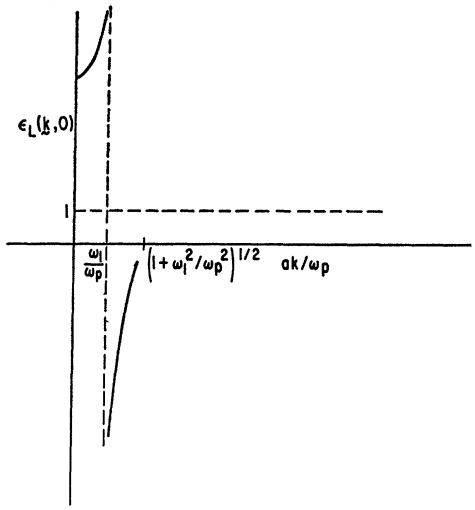

FIG. 4. The static dielectric constant of the Lorentz lattice as a function of wave vector k.

It follows from (3.11) that

$$\epsilon_L(0,\omega)=1-\omega_p^2/(\omega^2-\omega_1^2). \tag{3.12}$$

A plot of $\epsilon_L(0,\omega)$ against ω is shown in Fig. 3.

Case II: Static Response ($\omega=0$)

$$\frac{1}{\epsilon_L(\mathbf{k},0)}=1-\frac{\omega_p^2}{k^2}\sum_\lambda \frac{(\mathbf{k}\cdot\hat{\epsilon}_{\mathbf{k}\lambda})^2}{[\omega^2(\mathbf{k},\lambda)+\omega_1^2]}. \tag{3.13}$$

We consider, in particular, the long-wavelength case ($ak\ll\omega_p$) when only the longitudinal mode contributes to the sum over λ. The frequency of the longitudinal mode is given in Eq. (1.13). Using this in (3.13) one easily finds that

$$\epsilon_L(\mathbf{k},0)\rightarrow 1-\omega_p^2/(a^2k^2-\omega_1^2). \tag{3.14}$$

A plot of $\epsilon_L(\mathbf{k},0)$ against k for small k is shown in Fig. 4.

Comparison of Figs. 3 and 4 with Figs. 1 and 2 helps to explain some peculiar characteristics of the dielectric constant of the Wigner lattice. Its most striking feature is the fact that the static dielectric constant of the Wigner lattice is negative for all k, including in particular the long-wavelength limit. This is very different from the case of a normal insulator for which the long-wavelength static dielectric constant is positive. However, a study of Figs. 1–4 shows that no basic contradiction is involved here. In many cases a dipolar insulator can be represented fairly well by the Lorentz model. As expected, we find that in the Lorentz model the static, long-wavelength dielectric constant is finite and positive ($=1+\omega_p^2/\omega_1^2$). The Wigner crystal is basically a special case of the Lorentz model for which $\omega_1=0$ and $\omega_0=\omega_p/\sqrt{3}$. In that case, in Fig. 3 for example, the vertical dotted line moves to the left to coincide with the ordinate. So the portion of the curve to the left of the vertical dotted line disappears. In this way one passes smoothly from the stable Lorentz model to the limiting case of the Wigner crystal which is a lattice of electrons on the edge of instability.

IV. CONCLUSION

In this paper we have discussed the longitudinal dielectric property of the Wigner crystal. The most striking feature of the result is the fact that the dielectric constant for low $\mathbf{k}$ and small ω is negative. We have also pointed out that the Wigner lattice can be regarded as a limiting case of the classical Lorentz lattice just on the borderline of stability. The negative dielectric constant, occurring in certain frequency and wave-vector ranges (see Figs. 1–4) in both the Wigner and Lorentz lattices, indicates the possibility of an effective attractive force between two conduction electrons placed in such a lattice. One may speculate that this fact may find application in analyzing insulators which, when doped, become superconductors.[10]

ACKNOWLEDGMENTS

The author wishes to thank Professor W. Kohn for his constant guidance throughout the course of this work. Stimulating conversations with Professor P. Nozières are also gratefully acknowledged.

[10] An example is the substance studied by C. S. Koonce, M. L. Cohen, J. F. Schooley, W. R. Hosler, and E. R. Pfeiffer, Phys. Rev. **163**, 380 (1967).