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Some static and dynamical properties of a two-dimensional Wigner crystal*

Lynn Bonsall
IBM Thomas J. Watson Research Center, P. O. Box 218, Yorktown Heights, New York 10598

A. A. Maradudin†
Department of Physics, University of California, Irvine, California 92664
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The static ground-state energy of a two-dimensional Wigner crystal has been obtained for each of the five two-dimensional Bravais lattices. At constant electron number density the hexagonal lattice has the lowest energy. Phonon dispersion curves have been calculated for wave vectors along the symmetry directions in the first Brillouin zone for the hexagonal lattice. In the long-wavelength limit one of the two branches of the dispersion relation vanishes with vanishing two-dimensional wave vector $\vec{q}$ as q, the second as $q^{1/2}$. The coefficient of q in the former branch is pure imaginary for certain directions of propagation in the square lattice, implying a dynamical instability of this lattice; the hexagonal lattice is stable. The vibrational zero-point energy and low-temperature thermodynamic functions have been obtained for the hexagonal lattice. The dielectric susceptibility tensor of a two-dimensional Wigner crystal $\chi_{\alpha\beta}(\vec{q})$ has been determined in the long-wavelength limit, in the presence of a static magnetic field perpendicular to the crystal, and the result has been used to obtain the dispersion relation for plasma oscillations in the electron crystal.

I. INTRODUCTION

The possibility that a system of electrons in the presence of a compensating background of positive charge will crystallize in the low-density limit was first pointed out by Wigner in 1934.[1] Since that time a considerable body of work has been created devoted to one or another property of the three-dimensional Wigner crystal.[2] Recently, Chaplik[3] applied this idea to electrons or holes in inversion layers near the surface of a semiconductor. He pointed out that in a strong electric field at low temperatures the charge carriers can crystallize into a two-dimensional crystal and execute small vibrations about the resulting equilibrium position.

Alternatively, it has been proposed by Crandall and Williams[4] that a two-dimensional electron crystal can be created by the application of a strong electric field perpendicular to the free surface of liquid helium. In this case, the electron crystal resides just above the liquid surface. Recently, calculations of the frequency spectrum of such a system have been carried out.[5,6]

In the case that the system of inversion-layer electrons is a two-dimensional gas, the response of the gas to a longitudinal electric field was first calculated by Stern[7] using the self-consistent-field approximation. These results were used to obtain the plasmon dispersion relation for a two-dimensional electron gas embedded in a three-dimensional dielectric. Chiu and Quinn[8] generalized this work by calculating the response of a two-dimensional electron gas in the presence of a strong constant magnetic field applied in a direction normal to the plane of the gas. These results were used to obtain the dispersion relation of a magnetoplasma wave of a two-dimensional electron gas which occupies the plane $z = 0$ in a medium whose dielectric constant is ϵ_0.

In this paper, we assume the existence of a two-dimensional Wigner lattice and present the results of a study of several static and dynamical properties of such a lattice.

In Sec. II we calculate the static ground-state energy of the two-dimensional electron crystal for each of the five two-dimensional Bravais lattices. Phonon dispersion curves are obtained for wave vectors along the symmetry directions in the first Brillouin zone for the hexagonal lattice in Sec. III, and the vibrational zero-point energy is calculated for this lattice in Sec. IV.

In Sec. V, the phonon dispersion relation is obtained in the long-wavelength limit for the square and hexagonal lattices. The low-temperature thermodynamic functions are presented in Sec. VI for the hexagonal lattice. In Sec. VII, the dielectric susceptibility tensor is determined in the long-wavelength limit, in the presence of a static magnetic field perpendicular to the crystal, and in Sec. VIII, this result is used to obtain the dispersion relation for plasma oscillations in the electron crystal. Dispersion curves for several values of the cyclotron frequency are calculated, and the conclusions of our study of these dynamic properties are presented in Sec. IX.

Very recently, a paper by Meissner, Namaizawa, and Voss[9] appeared which is devoted to some of the properties of a two-dimensional Wigner crystal treated in this paper. The differences between the contents of these two works are that

Meissner *et al.* have calculated the static ground-state energy for only the triangular and square lattices, while it has been calculated for each of the two-dimensional Bravais lattices in the present work; Meissner *et al.* have obtained the dispersion curves for a three-layer structure, viz., metal-insulator-semiconductor, in which a triangular electron crystal is imbedded in the insulator-semiconductor interface, while we have ignored the metal layer in our work; in this paper we have obtained the dielectric susceptibility of a two-dimensional Wigner Bravais crystal, and have used the result to study the plasma oscillations of such a system.

II. STATIC GROUND-STATE ENERGY OF A WIGNER BRAVAIS CRYSTAL

When a two-dimensional electron gas crystallizes into a two-dimensional crystal it is natural to inquire about the structure this crystal possesses. In principle, this question can be answered by calculating the Helmholtz free energy at the absolute zero of temperature, at constant electron number density, for every possible structure the two-dimensional crystal can assume, and determining in this way the structure with the lowest energy. This is clearly an impossible task. In this section we pursue a much more limited goal. We calculate the static ground-state energy of a two-dimensional Wigner crystal, at constant electron number density, for each of the five two-dimensional Bravais lattices. The free energy of a Wigner crystal at the absolute zero of temperature is the sum of the static ground-state energy and the vibrational zero-point energy. A calculation of the latter, in the harmonic approximation, will be carried out in Sec. IV.

The lattice points of a two-dimensional Bravais lattice assumed to be in the xy plane, are given by the vectors

$$\vec{x}(l) = l_1\vec{a}_1 + l_2\vec{a}_2 , \tag{2.1}$$

where $\vec{a}_1$ and $\vec{a}_2$ are the primitive translation vectors of the lattice; and l_1 and l_2 are any two integers, positive, negative, or zero, to which we refer collectively as l.

We also define a lattice reciprocal to the direct lattice defined by Eq. (2.1) as the set of points given by the vectors

$$\vec{G}(h) = h_1\vec{b}_1 + h_2\vec{b}_2 , \tag{2.2}$$

where $\vec{b}_1$ and $\vec{b}_2$, are the primitive translation vectors of the reciprocal lattice. The primitive translation vectors $\vec{a}_1$, $\vec{a}_2$, $\vec{b}_1$, $\vec{b}_2$, and the area a_c of the primitive unit cell of the direct lattice are given in Table I for each of the five two-dimensional Bravais lattices.

The energy of interaction of a given electron (assumed to be at the origin of coordinates) with all the other electrons in the crystal can be expressed in the form

$$E_I^{(e)} = e^2 \lim_{\vec{x}\to 0}\left(\sum_l \frac{1}{|\vec{x}-\vec{x}(l)|} - \frac{1}{|\vec{x}|}\right), \tag{2.3}$$

where e is the magnitude of the electronic charge. In the case that the electron crystal is imbedded in a dielectric medium of dielectric constant ϵ_0 the electron's charge in this equation and in the results that follow from it should be replaced by $e/\epsilon_0^{1/2}$. With the aid of the integral representation

$$\frac{1}{|\vec{x}-\vec{x}(l)|} = \frac{1}{\sqrt{\pi}}\int_0^\infty dt\, t^{-1/2} e^{-t|\vec{x}-\vec{x}(l)|^2}, \tag{2.4}$$

and the two-dimensional form of Ewald's generalized theta function transformation

$$\sum_l \exp[-t|\vec{x}-\vec{x}(l)|^2 - i\vec{q}\cdot\vec{x}(l)] = \frac{\pi}{a_c t}\sum_{\vec{G}} \exp(i\vec{G}\cdot\vec{x}) \exp\left(-\frac{|\vec{q}+\vec{G}|^2}{4t}\right), \tag{2.5}$$

TABLE I. Five two-dimensional Bravais lattices.

Bravais lattice	$\vec{a}_1$	$\vec{a}_2$	$\vec{b}_1$	$\vec{b}_2$	a_c
Oblique	$(a,0)$	(c,b)	$2\pi\left(\frac{1}{a},-\frac{c}{ab}\right)$	$2\pi\left(0,\frac{1}{b}\right)$	ab
Primitive rectangular	$(a,0)$	$(0,b)$	$2\pi\left(\frac{1}{a},0\right)$	$2\pi\left(0,\frac{1}{b}\right)$	ab
Centered rectangular	$(a,0)$	$(\frac{1}{2}a,\frac{1}{2}b)$	$2\pi\left(\frac{1}{a},-\frac{1}{b}\right)$	$2\pi\left(0,\frac{2}{b}\right)$	$\frac{1}{2}ab$
Square	$(a_0,0)$	$(0,a_0)$	$\frac{2\pi}{a_0}(1,0)$	$\frac{2\pi}{a_0}(0,1)$	a_0^2
Hexagonal	$a_0(1,0)$	$a_0(\frac{1}{2},\frac{1}{2}\sqrt{3})$	$\frac{2\pi}{a_0}\left(1,-\frac{\sqrt{3}}{3}\right)$	$\frac{2\pi}{a_0}\left(0,\frac{2\sqrt{3}}{3}\right)$	$\frac{\sqrt{3}}{2}a_0^2$

we can reexpress $E_I^{(e)}$ in the form

$$E_I^{(e)} = \frac{2\pi e^2}{a_c}\left(\frac{1}{G}\right)_{\vec{G}=0} - \frac{2e^2}{a_c}\left(\frac{\pi}{\epsilon}\right)^{1/2} + \frac{e^2}{a_c}\left(\frac{\pi}{\epsilon}\right)^{1/2}\sum_{\vec{G}(\neq 0)} \varphi_{-1/2}\left(\frac{G^2}{4\epsilon}\right) - 2e^2\left(\frac{\epsilon}{\pi}\right)^{1/2} + e^2\left(\frac{\epsilon}{\pi}\right)^{1/2}\sum_{l\neq 0} \varphi_{-1/2}(\epsilon x^2(l)). \tag{2.6}$$

In this result ϵ is the usual separation parameter in the Ewald method,[10] and the right-hand side of Eq. (2.6) is independent of the value of this parameter. The $\{\varphi_n(z)\}$ are the Misra functions[11]

$$\varphi_n(z) = \int_1^\infty dt\, t^n e^{-zt}. \tag{2.7}$$

The singular first term on the right-hand side of Eq. (2.6) has its origin in the lack of charge neutrality in the electron lattice considered thus far.

To make our system electrically neutral, we assume that the two-dimensional Wigner crystal is embedded in a uniform two-dimensional background of positive charge, whose charge density is $\rho_+ = e/a_c$. The energy of interaction of our reference electron with this neutralizing background is

$$E_I^{(b)} = -e\rho_+ \int \frac{d^2x}{|\vec{x}|}. \tag{2.8}$$

If we use the two-dimensional Fourier expansion of $|\vec{x}|^{-1}$,

$$\frac{1}{|\vec{x}|} = \frac{2\pi}{L^2}\sum_{\vec{k}} \frac{1}{k} e^{i\vec{k}\cdot\vec{x}}, \tag{2.9}$$

where

$$\vec{k} = (2\pi/L)(n_x, n_y), \quad n_x, n_y = 0, \pm 1, \pm 2, \ldots \tag{2.10}$$

and L^2 is the area of the two-dimensional Wigner crystal, we obtain for $E_I^{(b)}$,

$$E_I^{(b)} = -\frac{2\pi e^2}{a_c}\frac{1}{L^2}\sum_{\vec{k}} \frac{1}{k}\int d^2x\, e^{i\vec{k}\cdot\vec{x}} = \frac{-2\pi e^2}{a_c}\left(\frac{1}{k}\right)_{\vec{k}=0}. \tag{2.11}$$

The total interaction energy is therefore given by

$$E_I = E_I^{(e)} + E_I^{(b)} = -\frac{2e^2}{a_c}\left(\frac{\pi}{\epsilon}\right)^{1/2} + \frac{e^2}{a_c}\left(\frac{\pi}{\epsilon}\right)^{1/2}\sum_{\vec{G}(\neq 0)} \varphi_{-1/2}\left(\frac{G^2}{4\epsilon}\right) - 2e^2\left(\frac{\epsilon}{\pi}\right)^{1/2} + e^2\left(\frac{\epsilon}{\pi}\right)^{1/2}\sum_{l(\neq 0)} \varphi_{-1/2}(\epsilon x^2(l)), \tag{2.12}$$

which is finite. The total static ground-state energy of the two-dimensional Wigner crystal is

$$E_G = \tfrac{1}{2}NE_I, \tag{2.13}$$

where $N = L^2/a_c$ is the number of electrons in the crystal, and the factor of $\frac{1}{2}$ accounts for the double counting of interactions in the calculation of E_G. The ground-state energy per electron is therefore $\frac{1}{2}E_I$.

The result (2.12) can be simplified considerably. If we use Eqs. (2.1), (2.2), and the results of Table I, we find that

$$\frac{G^2}{4\epsilon} = \frac{\pi^2}{\epsilon a_c^2}(h_2^2a_1^2 - 2h_1h_2\vec{a}_1\cdot\vec{a}_2 + h_1^2a_2^2), \tag{2.14a}$$

$$\epsilon x^2(l) = \epsilon(l_1^2a_1^2 + 2l_1l_2\vec{a}_1\cdot\vec{a}_2 + l_2^2a_2^2). \tag{2.14b}$$

Consequently, if we choose $\epsilon = \pi/a_c$, and change the dummy summation variables h_1, h_2 into $-l_2, l_1$, respectively, we obtain the simple result

$$E_I = -\frac{2e^2}{(a_c)^{1/2}}\left[2 - \sum_{l(\neq 0)} \varphi_{-1/2}\left(\frac{\pi}{a_c}x^2(l)\right)\right], \tag{2.15}$$

which is valid for any two-dimensional Wigner Bravais crystal. We consider each of these lattices in turn.

A. Oblique lattice

From Eq. (2.15) and Table I we find that the expression for the interaction energy for this lattice can be written

$$E_I(x,y) = -\frac{2e^2}{(a_c)^{1/2}} \times \left[2 - \sum_{l_1 l_2}{}' \varphi_{-1/2}\left(\frac{\pi}{x}[(l_1 + l_2y)^2 + l_2x^2]\right)\right], \tag{2.16}$$

where $x = b/a$, $y = c/a$, and $0 < y < 1$. Rather than evaluate this expression for all possible values of the parameters x and y, we consider the special cases which constitute the remaining two-dimensional lattices, starting with the most symmetric.

B. Square lattice

The interaction energy of the square lattice is given by

$$E_I = -\frac{2e^2}{a_0}\left(2 - \sum_{l_1 l_2}{}' \varphi_{-1/2}(\pi(l_1^2 + l_2^2))\right) = -3.900\,265\frac{e^2}{(a_c)^{1/2}}. \tag{2.17}$$

C. Hexagonal lattice

For the hexagonal lattice, we find that

$$E_I=\frac{-2\sqrt{2}}{3^{1/4}a_0}\left[2-\sum_{n_1n_2}{}'\varphi_{-1/2}\left(\frac{2\sqrt{3}}{3}\pi\,(n_1^2-n_1n_2+n_2^2)\right)\right]$$

$$=-3.921\,034\frac{e^2}{(a_c)^{1/2}}. \tag{2.18}$$

D. Primitive rectangular lattice

For the case of the primitive rectangular lattice

$$E_I(\lambda)=\frac{-2e^2}{(a_c)^{1/2}}\left(2-\sum_{l_1l_2}{}'\varphi_{-1/2}(\pi(\lambda l_1^2+\lambda^{-1}l_2^2))\right), \tag{2.19}$$

where $\lambda=a_1/a_2$. Note that for this lattice $E_I(\lambda)=E_I(1/\lambda)$. Thus we need to consider only the range $0<\lambda\leq 1$. If we choose $\lambda=0.95$, the interaction energy is given by

$$E_I(0.95)=-3.898\,597\,e^2/(a_c)^{1/2}, \tag{2.20}$$

which is higher than that of the square lattice. The lowest value of the energy for the primitive rectangular lattice is obtained for the limiting case $\lambda=1$, when the rectangular lattice becomes a square lattice.

E. Centered rectangular lattice

For this structure, the interaction energy becomes

$$E_I(\lambda)=\frac{-2e^2}{(a_c)^{1/2}}\left(2-\sum_{l_1l_2}{}'\varphi_{-1/2}\times\tfrac{1}{2}\pi[(2l_1+l_2)^2\lambda+l_2^2\lambda^{-1}]\right), \tag{2.21}$$

where $\lambda=a/b$, and again $E_I(\lambda)=E_I(1/\lambda)$. For $\lambda=1$, the energy of the centered rectangular lattice is equal to that of the square lattice. For $\lambda=0.95$, we find

$$E_I(0.95)=-3.900\,647\,e^2/(a_c)^{1/2}, \tag{2.22}$$

which is lower than that of the square lattice. A minimum in the interaction energy occurs at $\lambda=1/\sqrt{3}=0.577\,35\ldots$. For this value of λ the centered rectangular lattice becomes the hexagonal lattice.

Thus, from the results of these calculations, we conclude that the hexagonal lattice has the lowest energy of all the five two-dimensional Bravais lattices.

III. PHONON DISPERSION CURVES FOR A TWO-DIMENSIONAL WIGNER CRYSTAL

After the discussion of the static properties of a two-dimensional Wigner Bravais crystal in Sec. II we turn to a consideration of a dynamical property, viz., to a determination of the normal modes of vibration of such a crystal.

Whereas a three-dimensional Wigner crystal requires the presence of a uniform compensating background of positive charge for dynamical stability,[2d,2e] this is not the case for a two-dimensional Wigner crystal. For these crystals such a background makes no contribution to the dynamical matrix, and we will ignore it in what follows.

When each electron is given an arbitrary displacement $\vec{u}(l)$ from its equilibrium position $\vec{x}(l)$, the potential energy of the crystal is given by

$$\Phi=\frac{e^2}{2}\sum_{ll'}{}'\frac{1}{|\vec{x}(ll')+\vec{u}(ll')|}, \tag{3.1}$$

where we have used the notation

$$\vec{x}(ll')=\vec{x}(l)-\vec{x}(l'),\quad \vec{u}(ll')=\vec{u}(l)-\vec{u}(l'). \tag{3.2}$$

We now expand the potential energy in powers of the atomic displacements to second order:

$$\Phi=\Phi_0+\frac{1}{2}\sum_{l\alpha}\sum_{l'\beta}\Phi_{\alpha\beta}(ll')u_\alpha(l)u_\beta(l')+\cdots. \tag{3.3}$$

In this expression $\alpha,\beta=x,y$ label the Cartesian axes. The first-order term in this expansion vanishes because every electron is at a center of inversion. The atomic force constants $\{\Phi_{\alpha\beta}(ll')\}$ are given explicitly by

$$\Phi_{\alpha\beta}(ll')=-e^2\left(\frac{3x_\alpha(ll')x_\beta(ll')}{x^5(ll')}-\frac{\delta_{\alpha\beta}}{x^3(ll')}\right),\quad l\neq l' \tag{3.4a}$$

$$\Phi_{\alpha\beta}(ll)=e^2\sum_{l'(\neq l)}\left(\frac{3x_\alpha(ll')x_\beta(ll')}{x^5(ll')}-\frac{\delta_{\alpha\beta}}{x^3(ll')}\right). \tag{3.4b}$$

The Fourier transformed dynamical matrix $C_{\alpha\beta}(\vec{q})$, whose eigenvalues are the squares of the normal mode frequencies, is defined by

$$C_{\alpha\beta}(\vec{q})=\frac{1}{m^*}\sum_{l'}\Phi_{\alpha\beta}(ll')e^{-i\vec{q}\cdot\vec{x}(ll')}, \tag{3.5}$$

where m^* is the mass of an electron. In terms of the matrix

$$S_{\alpha\beta}(\vec{q})=\sum_{l'(\neq l)}\left(\frac{3x_\alpha(ll')x_\beta(ll')}{x^5(ll')}-\frac{\delta_{\alpha\beta}}{x^3(ll')}\right)e^{-i\vec{q}\cdot\vec{x}(ll')}, \tag{3.6}$$

we can express $C_{\alpha\beta}(\vec{q})$ as

$$C_{\alpha\beta}(\vec{q}) = -(e^2/m^*)[S_{\alpha\beta}(\vec{q}) - S_{\alpha\beta}(\vec{0})] . \tag{3.7}$$

We find that we can rewrite Eq. (3.6) equivalently as

$$S_{\alpha\beta}(\vec{q}) = \lim_{\vec{x}\to 0} \frac{\partial^2}{\partial x_\alpha \partial x_\beta} \left(e^{i\vec{q}\cdot\vec{x}} \sum_l \frac{e^{-i\vec{q}\cdot[\vec{x}-\vec{x}(l)]}}{|\vec{x}-\vec{x}(l)|} - \frac{1}{|\vec{x}|} \right) . \tag{3.8}$$

With the aid of Eqs. (2.4) and (2.5) we can transform this expression into the rapidly convergent form

$$S_{\alpha\beta}(\vec{q}) = \left(\frac{\pi}{\epsilon}\right)^{1/2} \frac{1}{a_c} \sum_{\vec{G}} (\vec{q}+\vec{G})_\alpha (\vec{q}+\vec{G})_\beta \varphi_{-1/2}\left(\frac{|\vec{q}+\vec{G}|^2}{4\epsilon}\right) + \frac{4}{3}\frac{\epsilon^{3/2}}{\pi^{1/2}}\delta_{\alpha\beta}$$

$$+ \left(\frac{\epsilon}{\pi}\right)^{1/2} \sum_{l(\neq 0)} e^{i\vec{q}\cdot\vec{x}(l)} \left[4\epsilon^2 x_\alpha(l) x_\beta(l) \varphi_{3/2}(\epsilon x^2(l)) - 2\epsilon\delta_{\alpha\beta}\varphi_{1/2}(\epsilon x^2(l))\right] . \tag{3.9}$$

The dynamical matrix $C_{\alpha\beta}(\vec{q})$ is obtained from $S_{\alpha\beta}(\vec{q})$ according to Eq. (3.7). In this way we obtain

$$C_{\alpha\beta}(\vec{q}) = \frac{2\pi e^2}{m^* a_c}\frac{q_\alpha q_\beta}{q} + \frac{2\pi e^2}{m^* a_c}\frac{q_\alpha q_\beta}{q}\left[\frac{q}{2(\pi\epsilon)^{1/2}}\varphi_{-1/2}\left(\frac{q^2}{4\epsilon}\right) - 1\right]$$

$$+ \frac{e^2}{m^* a_c}\left(\frac{\pi}{\epsilon}\right)^{1/2} \sum_{\vec{G}(\neq 0)} \left[(\vec{q}+\vec{G})_\alpha (\vec{q}+\vec{G})_\beta \varphi_{-1/2}\left(\frac{|q+G|^2}{4\epsilon}\right) - G_\alpha G_\beta \varphi_{-1/2}\left(\frac{G^2}{4\epsilon}\right)\right]$$

$$+ \frac{e^2}{m^*}\left(\frac{\epsilon}{\pi}\right)^{1/2} \sum_{l(\neq 0)} [1 - \cos\vec{q}\cdot\vec{x}(l)][4\epsilon^2 x_\alpha(l) x_\beta(l) \varphi_{3/2}(\epsilon x^2(l)) - 2\epsilon\delta_{\alpha\beta}\varphi_{1/2}(\epsilon x^2(l))] . \tag{3.10}$$

In writing this expression we have used the fact that every site is at a center of inversion in a Bravais lattice. We have also separated the dominant contribution to $C_{\alpha\beta}(\vec{q})$ in the limit of small $\vec{q}$ from the terms of higher order and have written it explicitly as the first term on the right-hand side of Eq. (3.10).

Earlier calculations of the phonon dispersion curves of two-dimensional Wigner lattices either did not transform the slowly convergent lattice sums $S_{\alpha\beta}(\vec{q})$ which enter the expression for the dynamical matrix $C_{\alpha\beta}(\vec{q})$ into rapidly convergent expressions,[6] or where this was done by means of the Ewald transformation, the results applied only to one Bravais lattice and contained typographical errors in the published expressions for $C_{\alpha\beta}(\vec{q})$.[5]

The normal mode frequencies of a two-dimensional Bravais crystal $\{\omega_j(\vec{q})\}$ are obtained from the solutions of the eigenvalue problem

$$\sum_\beta C_{\alpha\beta}(\vec{q}) e_\beta(\vec{q}j) = \omega_j^2(\vec{q}) e_\alpha(\vec{q}j) , \tag{3.11}$$

where $j = 1, 2$ labels the two solutions of Eq. (3.11) for each value of $\vec{q}$. Because $C_{\alpha\beta}(\vec{q})$ is a real, symmetric matrix the eigenvectors $\{e_\alpha(\vec{q}j)\}$ can be assumed to be orthonormal and complete. The values of the wave vector $\vec{q}$ can be restricted to lie inside the irreducible element of the two-dimensional first Brillouin zone of the crystal, from which the entire zone is generated by application of the operations of the point group of the Bravais lattice.

We have solved Eq. (3.11) for the hexagonal lattice for values of the wave vector $\vec{q}$ along the boundary of the irreducible element of the corresponding Brillouin zone depicted in Fig. 1. The dispersion curves so obtained are plotted in Fig. 2. We note that while the dispersion curves for the lower-frequency transverse branch vary linearly with the magnitude of the wave vector $\vec{q}$ in the limit as $\vec{q}\to 0$, the dispersion curves for the higher-frequency longitudinal branch tend to zero as $q^{1/2}$ in the limit as $\vec{q}\to 0$. The latter behavior has been noted previously,[3,5] and is shown in Sec. V to be a general property of the long-wavelength longitudinal modes of a two-dimensional Wigner Bravais crystal, independent of the particular

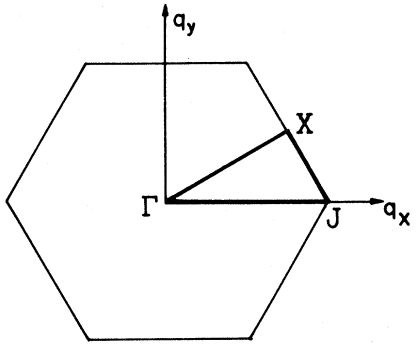

FIG. 1. First Brillouin zone for the two-dimensional, hexagonal lattice. The heavily outlined region is the irreducible element of this zone.

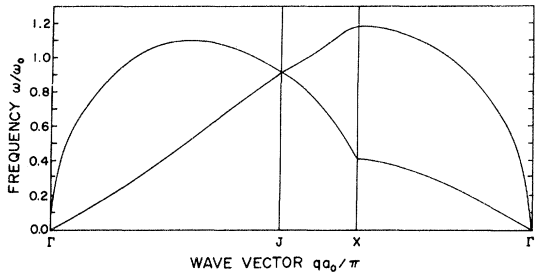

FIG. 2. Phonon dispersion curves for wave vectors along the boundary of the irreducible element of the first Brillouin zone for the two-dimensional hexagonal lattice. The frequency ω_0 is defined by $\omega_0^2 = 8e^2/m^* a_0^3 = 8(\sqrt{3}/4\pi)\omega_p^2$.

Bravais lattice under consideration. The results depicted in Fig. 2 will be discussed further in Sec. IX.

IV. ZERO-POINT ENERGY

We have already remarked that the first correction to the ground-state energy of a two-dimensional electron crystal comes from the zero-point energy of its vibrational motion. This is given by

$$E_0 = \tfrac{1}{2}\hbar \sum_{\vec{q}\, j} \omega_j(\vec{q}) , \tag{4.1}$$

where the sum on $\vec{q}$ is over the values in the two-dimensional first Brillouin zone allowed by periodic boundary conditions. We now replace summation over $\vec{q}$ by integration to obtain

$$E_0 = \frac{N\hbar}{2} \sum_j \frac{1}{a_{BZ}} \int_{BZ} \omega_j(\vec{q})\, d^2q , \tag{4.2}$$

where N is the number of primitive unit cells in the crystal, and

$$a_{BZ} = (2\pi)^2/a_c \tag{4.3}$$

is the area of the Brillouin zone. The integral over $\vec{q}$ is taken over the area of this zone.

The quantity

$$\langle \omega_j(\vec{q}) \rangle = \frac{1}{a_{BZ}} \int_{BZ} \omega_j(\vec{q})\, d^2q \tag{4.4}$$

is the average of $\omega_j(\vec{q})$ over the Brillouin zone. We have chosen to express the zero-point energy in the form

$$E_0 = \frac{N\hbar}{2} \sum_j \langle \omega_j(\vec{q}) \rangle , \tag{4.5}$$

because an efficient method has been developed recently for the evaluation of averages such as $\langle \omega_j(\vec{q}) \rangle$ of functions which possess the periodicity of the two-dimensional reciprocal lattice.[12] This method expresses $\langle \omega_j(\vec{q}) \rangle$ in the form

$$\langle \omega_j(\vec{q}) \rangle = \sum_{i=1}^{N} \alpha_i \omega_j(\vec{q}_i) , \tag{4.6}$$

where the weights $\{\alpha_i\}$ and the special values of the wave vector $\vec{q}$, $\{\vec{q}_i\}$, are tabulated in Ref. 12.

We have used this method, with $N = 6$, to evaluate the zero-point energy of the hexagonal crystal, using the results of Sec. III for the evaluation of the frequencies $\{\omega_j(\vec{q}_i)\}$. The result is

$$E_0 = \tfrac{1}{2} N\hbar (e^2/m^* a_0^3)^{1/2} (4.28) . \tag{4.7}$$

Greater accuracy in the evaluation of the zero-point energy is achievable through the use of a larger number of special points $\{\vec{q}_i\}$. It was not felt to be called for in the present work.

V. LONG-WAVELENGTH LIMIT

The results of Sec. III enable the normal mode frequencies of an arbitrary two-dimensional Wigner Bravais crystal to be obtained for an arbitrary wave vector $\vec{q}$ in the two-dimensional first Brillouin zone of the crystal. The somewhat complicated expressions for the elements of the dynamical matrix $C_{\alpha\beta}(\vec{q})$ simplify in the long-wavelength limit, i.e., in the limit as $\vec{q} \to 0$. This is an interesting limit to consider because it yields the speed of sound for the transverse branch of the phonon spectrum, which provides information about the dynamical stability of the corresponding lattice, and because the results obtained in this limit are useful in determining the dielectric susceptibility of a two-dimensional Wigner crystal (see Sec. VII). In this section we obtain the forms of the phonon dispersion curves to $O(q^2)$ for an arbitrary two-dimensional Wigner Bravais crystal.

We begin by writing the elements of the dynamical matrix $C_{\alpha\beta}(\vec{q})$ in the form

$$C_{\alpha\beta}(\vec{q}) = \frac{2\pi e^2}{m^* a_c} \frac{q_\alpha q_\beta}{q} + \bar{C}_{\alpha\beta}(\vec{q}) , \tag{5.1}$$

where, from Eq. (3.10),

$$\bar{C}_{\alpha\beta}(\vec{q}) = \frac{2\pi e^2}{m^* a_c} \frac{q_\alpha q_\beta}{q} \left[\frac{q}{2(\pi\epsilon)^{1/2}} \varphi_{-1/2}\left(\frac{q^2}{4\epsilon}\right) - 1 \right] + \frac{e^2}{m^* a_c} \left(\frac{\pi}{\epsilon}\right)^{1/2} \sum_{\vec{G}(\neq 0)} \left[(\vec{q}+\vec{G})_\alpha (\vec{q}+\vec{G})_\beta \varphi_{-1/2}\left(\frac{|\vec{q}+\vec{G}|^2}{4\epsilon}\right) - G_\alpha G_\beta \varphi_{-1/2}\left(\frac{G^2}{4\epsilon}\right) \right]$$

$$+ \frac{e^2}{m^*} \left(\frac{\epsilon}{\pi}\right)^{1/2} \sum_{l(\neq 0)} [1 - \cos \vec{q}\cdot\vec{x}(l)] [4\epsilon^2 x_\alpha(l) x_\beta(l) \varphi_{3/2}(\epsilon x^2(l)) - 2\epsilon \delta_{\alpha\beta} \varphi_{1/2}(\epsilon x^2(l))] = \bar{C}_{\alpha\beta}(-\vec{q}) . \tag{5.2}$$

We now use the results that for small q

$$\varphi_{-1/2}(q^2/4\epsilon) = 2(\pi\epsilon)^{1/2}/q - 2 + \tfrac{2}{3}q^2/4\epsilon - \tfrac{1}{5}q^4/16\epsilon^2 + \cdots , \tag{5.3a}$$

$$\varphi_{-1/2}\left(\frac{|\vec{q}+\vec{G}|^2}{4\epsilon}\right) = \varphi_{-1/2}\left(\frac{G^2}{4\epsilon}\right) - \frac{\vec{G}\cdot\vec{q}}{2\epsilon}\varphi_{1/2}\left(\frac{G^2}{4\epsilon}\right) + \frac{(\vec{G}\cdot\vec{q})^2}{8\epsilon^2}\varphi_{3/2}\left(\frac{G^2}{4\epsilon}\right) - \frac{q^2}{4\epsilon}\varphi_{1/2}\left(\frac{G^2}{4\epsilon}\right) + O(q^3) , \tag{5.3b}$$

to expand $\overline{C}_{\alpha\beta}(\vec{q})$ in powers of the components of the wave vector $\vec{q}$:

$$\overline{C}_{\alpha\beta}(\vec{q}) = C^{(2)}_{\alpha\beta}(\vec{q}) + C^{(4)}_{\alpha\beta}(\vec{q}) + \cdots , \tag{5.4}$$

where the superscripts denote the order of the corresponding terms in the components of $\vec{q}$. (The terms of odd order vanish identically because each lattice site is a center of inversion in a Bravais lattice.) The elements of the matrix $C^{(2)}_{\alpha\beta}(\vec{q})$, which is the only term in the expansion (5.4) with which we will be concerned here, are given by

$$C^{(2)}_{\alpha\beta}(\vec{q}) = \sum_{\mu\nu} A_{\alpha\beta\mu\nu} q_\mu q_\nu , \tag{5.5}$$

where

$$\begin{aligned} A_{\alpha\beta\mu\nu} = &-\frac{e^2}{4m^*a_c}\frac{\pi^{1/2}}{\epsilon^{3/2}}\delta_{\mu\nu}\sum_{\vec{G}(\neq 0)} G_\alpha G_\beta \varphi_{1/2}\left(\frac{G^2}{4\epsilon}\right) - \frac{e^2}{2m^*a_c}\left(\frac{\pi}{\epsilon}\right)^{1/2}(\delta_{\alpha\mu}\delta_{\beta\nu}+\delta_{\alpha\nu}\delta_{\beta\mu})\left[2 - \sum_{\vec{G}(\neq 0)}\varphi_{-1/2}\left(\frac{G^2}{4\epsilon}\right)\right] \\ &- \frac{e^2}{2m^*a_c}\frac{\pi^{1/2}}{\epsilon^{3/2}}\sum_{\vec{G}(\neq 0)}(G_\alpha G_\mu\delta_{\beta\nu} + G_\alpha G_\nu\delta_{\beta\mu} + G_\beta G_\mu\delta_{\alpha\nu} + G_\beta G_\nu\delta_{\alpha\mu})\varphi_{1/2}\left(\frac{G^2}{4\epsilon}\right) \\ &+ \frac{e^2}{8m^*a_c}\frac{\pi^{1/2}}{\epsilon^{5/2}}\sum_{\vec{G}(\neq 0)} G_\alpha G_\beta G_\mu G_\nu \varphi_{3/2}\left(\frac{G^2}{4\epsilon}\right) \\ &+ \frac{e^2}{2m^*}\left(\frac{\epsilon}{\pi}\right)^{1/2}\sum_{l(\neq 0)}[4\epsilon^2 x_\alpha(l)x_\beta(l)x_\mu(l)x_\nu(l)\varphi_{3/2}(\epsilon x^2(l)) - 2\epsilon\delta_{\alpha\beta}x_\mu(l)x_\nu(l)\varphi_{1/2}(\epsilon x^2(l))] . \end{aligned} \tag{5.6}$$

The elements of the tensor $A_{\alpha\beta\mu\nu}$ possess the following symmetry properties under interchanges of their subscripts:

$$A_{\alpha\beta\mu\nu} = A_{\beta\alpha\mu\nu} = A_{\alpha\beta\nu\mu} . \tag{5.7}$$

Furthermore, if $R_{\alpha\beta}$ is a 2×2 real, orthogonal matrix representative of a proper or improper (active) rotation in the xy plane that sends the two-dimensional Bravais lattice into itself, then $A_{\alpha\beta\mu\nu}$ is invariant under such a rotation in the sense that

$$A_{\alpha\beta\mu\nu} = \sum_{\alpha'\beta'\mu'\nu'} R_{\alpha\alpha'}R_{\beta\beta'}R_{\mu\mu'}R_{\nu\nu'}A_{\alpha'\beta'\mu'\nu'} . \tag{5.8}$$

We now regard the matrix $C^{(2)}_{\alpha\beta}(\vec{q})$ as a perturbation on the matrix

$$C^{(1)}_{\alpha\beta}(\vec{q}) = (2\pi e^2/m^*a_c)q_\alpha q_\pi/q . \tag{5.9}$$

The eigenvalues and (normalized) eigenvectors of this matrix are readily found to be

$$\omega^2_{01}(\vec{q}) = \frac{2\pi e^2}{m^*a_c}q , \quad \vec{V}(1) = \left(\frac{q_x}{q},\frac{q_y}{q}\right), \tag{5.10a}$$

$$\omega^2_{02}(\vec{q}) = 0 , \quad \vec{V}(2) = \left(\frac{q_y}{q},-\frac{q_x}{q}\right). \tag{5.10b}$$

We pause to note that the results given by Eqs. (5.10) have a general character in the sense that they are independent of the particular Bravais lattice for which the dispersion curves are being calculated. This is not true of the corrections to these results of higher order in the components of $\vec{q}$, which differ depending on the Bravais lattice being studied. First-order nondegenerate perturbation theory suffices to obtain the corrections to these eigenvalues arising from the matrix $C^{(2)}_{\alpha\beta}(\vec{q})$. Indeed, we have

$$\Delta\omega^2_1(\vec{q}) = \frac{1}{q^2}\sum_{\alpha\beta\mu\nu} A_{\alpha\beta\mu\nu}q_\alpha q_\beta q_\mu q_\nu \tag{5.11}$$

and

$$\Delta\omega^2_2(\vec{q}) = \sum_{\alpha\mu\nu} A_{\alpha\alpha\mu\nu}q_\mu q_\nu - \Delta\omega^2_1(\vec{q}) . \tag{5.12}$$

This is about as far as one can go, in general. We now specialize these general results to the square and hexagonal lattices.

A. Square lattice

In this case, Eqs. (5.8) and (5.9), together with the operations of the point group C_{4v}, lead to the

result that there are only three independent nonzero elements of the tensor $A_{\alpha\beta\mu\nu}$. These are A_{xxxx}, A_{xxyy}, and A_{xyxy}. If we use Eqs. (2.1), (2.2), (2.23), (2.24), and the results in Table I, we obtain, for these coefficients,

$$A_{xxxx} = (e^2/m^*a_0)(-0.828\,777)\,, \tag{5.13}$$

$$A_{xxyy} = (e^2/m^*a_0)(-0.146\,289)\,, \tag{5.14}$$

$$A_{xyxy} = (e^2/m^*a_0)(-1.121\,356)\,. \tag{5.15}$$

The elements of the matrix $C^{(2)}_{\alpha\beta}(\vec{q})$ are therefore given by

$$C^{(2)}_{xx}(\vec{q}) = (-e^2/m^*a_0) \times (0.828\,777q_x^2 + 0.146\,289q_y^2)\,, \tag{5.16a}$$

$$C^{(2)}_{xy}(\vec{q}) = C^{(2)}_{yx}(\vec{q}) = (-e^2/m^*a_0)(2.242\,712q_xq_y)\,, \tag{5.16b}$$

$$C^{(2)}_{yy}(\vec{q}) = (-e^2/m^*a_0)(0.146\,289q_x^2 + 0.828\,777q_y^2)\,. \tag{5.16c}$$

From these results and Eqs. (5.11)–(5.12) we find for the corrections to the normal mode frequencies of $O(q^2)$,

$$\Delta\omega_1^2(\vec{q}) = -\omega_0^2(a_0q)^2 \times (0.131\,904 + 0.496\,635\hat{q}_x^2\hat{q}_y^2)\,, \tag{5.17a}$$

$$\Delta\omega_2^2(\vec{q}) = \omega_0^2(a_0q)^2 \times (-0.023\,282\,6 + 0.496\,635\hat{q}_x^2\hat{q}_y^2)\,, \tag{5.17b}$$

where we have introduced the notation $\omega_0^2 = 2\pi e^2/m^*a_0^3$. If we add these results to those given by Eq. (5.10), we find that through terms of $O(q^2)$,

$$\omega_1^2(\vec{q}) = \omega_0^2(a_0q) - \omega_0^2(a_0q)^2 \times (0.131\,904 + 0.496\,635\hat{q}_x^2\hat{q}_y^2)\,, \tag{5.18a}$$

$$\omega_2^2(\vec{q}) = \omega_0^2(a_0q)^2 \times (-0.023\,282\,6 + 0.496\,635\hat{q}_x^2\hat{q}_y^2)\,. \tag{5.18b}$$

We see that $\omega_2^2(\vec{q})$ is negative for certain directions of $\vec{q}$ (e.g., the [10] direction). Thus we have the result that for small q the frequency of the transverse branch $\omega_2(\vec{q})$ is pure imaginary for these directions of $\vec{q}$, implying an instability of the two-dimensional square Wigner crystal.[13] This result is in disagreement with that of earlier work[5] which showed that $\omega_2(\vec{q})$ is real for $\vec{q}$ along the [10] direction.

The fact that the two-dimensional square lattice is unstable is not too surprising. It is known[14] that a simple cubic lattice in three dimensions in which the particles interact with central forces only is unstable against shear. The result we have established is the two-dimensional analog of that result.

B. Hexagonal lattice

For the hexagonal lattice, Eqs. (5.8) and (5.9) together with the operations of the point group C_{6v}, lead to the result that there are only two independent nonzero elements of the tensor $A_{\alpha\beta\mu\nu}$. These are A_{xxxx} and A_{xxyy}, with $A_{xyxy} = \frac{1}{2}(A_{xxxx} - A_{xxyy})$. If we use Eqs. (2.1)–(2.5), (2.23), (2.24), and the results in Table I, we find we can write these coefficients as

$$A_{xxxx} = [e^2/m^*(a_c)^{1/2}](-1.225\,323)\,, \tag{5.19}$$

$$A_{xxyy} = [e^2/m^*(a_c)^{1/2}](0.245\,065)\,. \tag{5.20}$$

The elements of the matrix $C^{(2)}_{\alpha\beta}(\vec{q})$ are therefore given by

$$C^{(2)}_{xx}(\vec{q}) = [e^2/m^*(a_c)^{1/2}] \times (-1.225\,323q_x^2 + 0.245\,065q_y^2)\,, \tag{5.21a}$$

$$C^{(2)}_{xy}(\vec{q}) = C^{(2)}_{yx}(\vec{q}) = [e^2/m^*(a_c)^{1/2}](-1.470\,388q_xq_y)\,, \tag{5.21b}$$

$$C^{(2)}_{yy}(\vec{q}) = [e^2/m^*(a_c)^{1/2}] \times (0.245\,065q_x^2 - 1.225\,323q_y^2)\,. \tag{5.21c}$$

From these results and Eqs. (5.11) and (5.12), we find, for the corrections to the normal mode frequencies of $O(q^2)$,

$$\Delta\omega_1^2(\vec{q}) = -\omega_p^2(0.181\,483)(a_0q)^2\,, \tag{5.22a}$$

$$\Delta\omega_2^2(\vec{q}) = \omega_p^2(0.036\,296\,7)(a_0q)^2\,, \tag{5.22b}$$

where we have defined

$$2\pi e^2/m^*a_c = \omega_p^2a_0\,. \tag{5.23}$$

When we add these results to those given by Eq. (5.10), we find that through terms of $O(q^2)$,

$$\omega_1^2(\vec{q}) = \omega_p^2(a_0q) - \omega_p^2(0.181\,483)(a_0q)^2\,, \tag{5.24a}$$

$$\omega_2^2(\vec{q}) = \omega_p^2(0.036\,296\,7)(a_0q)^2\,. \tag{5.24b}$$

We see that for the hexagonal lattice the frequency of the transverse branch is real in the long-wavelength limit. Consequently, the hexagonal lattice, unlike the square lattice, is stable in this limit. In addition, these frequencies are isotropic, in the sense that they depend on q_x and q_y only in the combination $(q_x^2 + q_x^2)^{1/2}$.

VI. LOW-TEMPERATURE THERMODYNAMIC FUNCTIONS OF A TWO-DIMENSIONAL WIGNER CRYSTAL

The frequency distribution function (frequency spectrum) $g(\omega)$ of a two-dimensional Wigner

Bravais crystal can be written[15]

$$g(\omega)=\frac{1}{2N}\sum_{\vec{q}\,j}\delta(\omega-\omega_j(\vec{q}))\,, \tag{6.1}$$

where N is the number of electrons, and the sum on $\vec{q}$ is over the values in the two-dimensional Brillouin zone allowed by periodic boundary conditions.

The results of Sec. V enable us to obtain $g(\omega)$ in the limit of small ω for the hexagonal lattice, which suffices for a calculation of the thermodynamic functions of this lattice in the low-temperature limit. From Eqs. (5.25) we find that for this lattice

$$\omega_1(\vec{q})=\omega_p(a_0q)^{1/2}[1-0.09074(a_0q)]\,, \tag{6.2a}$$

$$\omega_2(\vec{q})=\omega_p(0.1905)(a_0q)\,. \tag{6.2b}$$

The dominant contribution to $g(\omega)$ in the limit as $\omega\to 0$ comes from the branch $\omega_2(\vec{q})$ in the present case, because the frequency of this branch vanishes with vanishing q according to the largest power of this wave vector. Thus, if we replace summation over $\vec{q}$ in Eq. (6.1) by integration, and use Eq. (6.2b), we find that

$$g(\omega)=\frac{a_c}{4\pi}\int dq\,q\,\delta(\omega-0.1905\omega_p(a_0q))+O(\omega^3)$$

$$=\frac{1}{4\pi(0.1905)^2}\frac{a_c}{\omega_p^2a_0^2}\omega+O(\omega^3)\,, \tag{6.3}$$

where the estimate of the remainder is made on the basis of the leading term neglected in the expression for $\omega_2(\vec{q})$ [of $O(q^3)$] and of the leading term in $\omega_1(\vec{q})$ [of $O(q^{1/2})$]. This result is exact in the limit of small ω.

Use of Eq. (6.3) enables us to obtain the leading term in the low-temperature expansion of the thermodynamic functions of the electron crystal. For example, the specific heat at constant volume is given by

$$C_v(T)=2Nk_B\int_0^{\omega_L}d\omega\,g(\omega)\left(\frac{\hbar\omega}{2k_BT}\right)^2$$

$$\times\left[\sinh^2\left(\frac{\hbar\omega}{2k_BT}\right)\right]^{-1}\,, \tag{6.4}$$

where ω_L is the largest normal mode frequency of the crystal. In the low-temperature limit this expression becomes

$$C_v(T)=\frac{3Nk_B}{\pi(0.1905)^2}\frac{a_c}{a_0^2}\left(\frac{k_BT}{\hbar\omega_p}\right)^2\zeta(3)+O(T^4)\,, \tag{6.5}$$

where $\zeta(3)$ is the Riemann zeta function. This result has the proportionality to T^2 characteristic of the low-temperature specific heat of a two-dimensional vibrational system.[16]

VII. DIELECTRIC SUSCEPTIBILITY OF A TWO-DIMENSIONAL WIGNER CRYSTAL

In this section we obtain the dielectric susceptibility of the two-dimensional Wigner crystal. It is straightforward to carry out this determination for the case that a static, external magnetic field is present, directed normal to the plane of the crystal, and we make this assumption here.

If we assume for the external magnetic field the form

$$\vec{B}=(0,0,B)\,, \tag{7.1}$$

the equations of motion of the two-dimensional Wigner crystal become ($\alpha,\beta=x,y$)

$$m^*\ddot{u}_\alpha(l)=-\sum_{l'\beta}\Phi_{\alpha\beta}(ll')u_\beta(l')$$

$$-\frac{eB}{c}\sum_\beta\epsilon_{\alpha\beta z}u_\beta(l)\,. \tag{7.2}$$

In these equations $\epsilon_{\alpha\beta\gamma}$ is the Levi-Civita tensor.

We assume a solution of the form

$$u_\alpha(l)=[W_\alpha(\vec{k}\omega)/\sqrt{m^*}]e^{i\vec{k}\cdot\vec{x}(l)-i\omega t}\,, \tag{7.3}$$

and obtain as the equations for the amplitudes $\{W_\alpha(\vec{k}\omega)\}$,

$$\omega^2W_\alpha(\vec{k}\omega)=\sum_\beta C_{\alpha\beta}(\vec{k})W_\beta(\vec{k}\omega)$$

$$-i\omega\omega_c\sum_\beta\epsilon_{\alpha\beta z}W_\beta(\vec{k}\omega)\,, \tag{7.4}$$

where the dynamical matrix $C_{\alpha\beta}(\vec{k})$ has been defined formally by Eq. (3.5), and a rapidly convergent expansion for it is given by Eq. (3.10). The frequency ω_c is the cyclotron frequency (eB/m^*c). If we substitute Eq. (5.1) into Eq. (7.4), and rearrange terms, we can write the result as

$$\omega^2W_\alpha(\vec{k}\omega)-\sum_\beta\overline{C}_{\alpha\beta}(\vec{k})W_\beta(\vec{k}\omega)+i\omega\omega_c\sum_\beta\epsilon_{\alpha\beta z}W_\beta(\vec{k}\omega)$$

$$=\frac{2\pi e^2}{m^*a_c}\sum_\beta\frac{k_\alpha k_\beta}{k}W_\beta(\vec{k}\omega)\,. \tag{7.5}$$

Our reason for writing the equations of motion in this fashion is that the right-hand side of this equation can be identified as arising from the force exerted on each electron by the macroscopic electric field in our system. This field, in fact, is established by the long-wavelength vibrations of the two-dimensional Wigner crystal.

To see this we note that the Coulomb field at the point $\vec{x}$ due to the presence of a dipole at each lattice site of a two-dimensional Bravais lattice is given by

$$E_\alpha^{\mathrm{Coul}}(\vec{x}) = \sum_{l'\beta} \frac{\partial^2}{\partial x_\alpha \partial x_\beta} \frac{1}{|\vec{x} - \vec{x}(l')|} p_\beta(l') , \tag{7.6}$$

where $\vec{p}(l)$ is the dipole moment at the lth lattice site. If we assume that the dipole moment varies from site to site and with time according to

$$p_\alpha(l) = p_\alpha(\vec{k}\omega) e^{i\vec{k}\cdot\vec{x}(l) - i\omega t} \tag{7.7}$$

and use the two-dimensional Fourier expansion of $|\vec{x}|^{-1}$, Eq. (2.9), we can rewrite the Coulomb field in the form

$$E_\alpha^{\mathrm{Coul}}(\vec{x}) = -\frac{2\pi}{a_c} e^{-i\omega t} \sum_\beta p_\beta(\vec{k}\omega) \times \sum_{\vec{G}} \frac{(\vec{k}+\vec{G})_\alpha (\vec{k}+\vec{G})_\beta}{|\vec{k}+\vec{G}|} e^{i(\vec{k}+\vec{G})\cdot\vec{x}} . \tag{7.8}$$

In the limit of small $|\vec{k}|$, which is the case of interest here, the term with $\vec{G} = 0$ in this expression gives the contribution to the electric field in the crystal which varies very slowly from unit cell to unit cell, while the terms with $\vec{G} \neq 0$ give the contributions to the field which vary rapidly over the area of each unit cell. Their spatial average over the area of any unit cell also vanishes in the small-$|\vec{k}|$ limit. The macroscopic electric field in the crystal is therefore given by

$$E_\alpha^M(\vec{x}) = E_\alpha(\vec{k}\omega) e^{i\vec{k}\cdot\vec{x} - i\omega t} , \tag{7.9}$$

with

$$E_\alpha(\vec{k}\omega) = -\frac{2\pi}{a_c} \sum_\beta \frac{k_\alpha k_\beta}{k} p_\beta(\vec{k}\omega) . \tag{7.10}$$

Now, if the lth electron is given a displacement $u_\alpha(l)$ from its equilibrium position, the dipole moment induced at that site is

$$\begin{aligned} p_\alpha(l) &= -eu_\alpha(l) \\ &= -e[W_\alpha(\vec{k}\omega)/\sqrt{m^*}] e^{i\vec{k}\cdot\vec{x}(l) - i\omega t} . \end{aligned} \tag{7.11}$$

Comparison of Eqs. (7.7) and (7.11) shows that in this case

$$p_\alpha(\vec{k}\omega) = -eW_\alpha(\vec{k}\omega)/\sqrt{m^*} . \tag{7.12}$$

The amplitude of the macroscopic field $E_\alpha(\vec{k}\omega)$, Eq. (7.10), established by the atomic motions is therefore

$$E_\alpha(\vec{k}\omega) = \frac{2\pi e}{a_c \sqrt{m^*}} \sum_\beta \frac{k_\alpha k_\beta}{k} W_\beta(\vec{k}\omega) . \tag{7.13}$$

We now return to Eq. (7.5) and use the result expressed by Eq. (7.13) in it to obtain

$$\omega^2 W_\alpha(\vec{k}\omega) - \sum_\beta \bar{C}_{\alpha\beta}(\vec{k}) W_\beta(\vec{k}\omega) + i\omega\omega_c \sum_\beta \epsilon_{\alpha\beta z} W_\beta(\vec{k}\omega) = \frac{e}{\sqrt{m^*}} E_\alpha(\vec{k}\omega) . \tag{7.14}$$

These are the time-independent equations of motion of a two-dimensional crystal composed of charges driven by an external electric field, in the presence of a static external magnetic field.

Equation (7.14) is readily solved to yield the relation between the amplitudes $W_\alpha(\vec{k}\omega)$ and $E_\alpha(\vec{k}\omega)$:

$$\begin{pmatrix} W_x(\vec{k}\omega) \\ W_y(\vec{k}\omega) \end{pmatrix} = \frac{e}{\sqrt{m^* D(\vec{k}\omega)}} \times \begin{pmatrix} \omega^2 - \bar{C}_{yy}(\vec{k}) & \bar{C}_{xy}(\vec{k}) - i\omega\omega_c \\ \bar{C}_{xy}(\vec{k}) + i\omega\omega_c & \omega^2 - \bar{C}_{xx}(\vec{k}) \end{pmatrix} \times \begin{pmatrix} E_x(\vec{k}\omega) \\ E_y(\vec{k}\omega) \end{pmatrix} , \tag{7.15}$$

where

$$\begin{aligned} D(\vec{k}\omega) = \omega^4 &- \omega^2[\bar{C}_{xx}(\vec{k}) + \bar{C}_{yy}(\vec{k}) + \omega_c^2] \\ &+ \bar{C}_{xx}(\vec{k})\bar{C}_{yy}(\vec{k}) - \bar{C}_{xy}^2(\vec{k}) , \end{aligned} \tag{7.16}$$

and use has been made of the symmetry relation $\bar{C}_{xy}(\vec{k}) = \bar{C}_{yx}(\vec{k})$.

The polarization in the two-dimensional crystal due to the electronic displacements is

$$\begin{aligned} P_\alpha(\vec{x}) &= \sum_l p_\alpha(l) \delta(\vec{x} - \vec{x}(l)) \\ &= p_\alpha(\vec{k}\omega) e^{i\vec{k}\cdot\vec{x} - i\omega t} \frac{1}{a_c} \sum_{\vec{G}} e^{i\vec{G}\cdot\vec{x}} . \end{aligned} \tag{7.17}$$

In the limit of small $|\vec{k}|$ it is the $\vec{G} = 0$ term in this sum which gives the macroscopic polarization in the crystal

$$P_\alpha^M(\vec{x}) = P_\alpha(\vec{k}\omega) e^{i\vec{k}\cdot\vec{x} - i\omega t} , \tag{7.18}$$

where

$$P_\alpha(\vec{k}\omega) = \frac{1}{a_c} p_\alpha(\vec{k}\omega) = -\frac{eW_\alpha(\vec{k}\omega)}{\sqrt{m^* a_c}} , \tag{7.19}$$

and where the latter expression applies to the amplitude of the macroscopic polarization created by the displacements of the electrons from their equilibrium positions.

If we substitute the expressions for $W_\alpha(\vec{k}\omega)$ given by Eq. (7.15) into Eq. (7.19), the result can be written in the form

$$P_\alpha(\vec{k}\omega) = \sum_\beta \chi_{\alpha\beta}^{(e)}(\vec{k}\omega) E_\beta(\vec{k}\omega) , \tag{7.20}$$

where the elements of the susceptibility tensor $\chi_{\alpha\beta}^{(e)}(\vec{k}\omega)$ are given explicitly by

$$\chi_{xx}^{(e)}(\vec{k}\omega) = -\frac{e^2}{m^* a_c}\frac{\omega^2 - \bar{C}_{yy}(\vec{k})}{D(\vec{k}\omega)}, \tag{7.21a}$$

$$\chi_{xy}^{(e)}(\vec{k}\omega) = \chi_{yx}^{(e)}(\vec{k}\omega)^* = -\frac{e^2}{m^* a_c}\frac{\bar{C}_{xy}(\vec{k}) - i\omega\omega_c}{D(\vec{k}\omega)}, \tag{7.21b}$$

$$\chi_{yy}^{(e)}(\vec{k}\omega) = -\frac{e^2}{m^* a_c}\frac{\omega^2 - \bar{C}_{xx}(\vec{k})}{D(\vec{k}\omega)}. \tag{7.21c}$$

We can use these expressions, together with the results of Sec. V, to write out explicitly the elements of the susceptibility tensor for a hexagonal crystal in the long-wavelength limit. For this we approximate the elements of the matrix $\bar{C}_{\alpha\beta}(\vec{k})$ by the elements of the matrix $C_{\alpha\beta}^{(2)}(\vec{k})$, which are given for this case by Eqs. (5.21). In this way we obtain

$$\chi_{xx}^{(e)}(\vec{k}\omega) = -\frac{\omega_p^2 a_0}{2\pi}\frac{\omega^2 - \omega_p^2(0.036\,297\xi_x^2 - 0.181\,48\xi_y^2)}{\omega^4 + \omega^2(0.1452\omega_p^2\xi^2 - \omega_c^2) - 0.006\,587\omega_p^4\xi^4}, \tag{7.22a}$$

$$\chi_{xy}^{(e)}(\vec{k}\omega) = \chi_{yx}^{(e)}(\vec{k}\omega)^* = -\frac{\omega_p^2 a_0}{2\pi}\frac{-\omega_p^2(0.217\,780)\xi_x\xi_y - i\omega\omega_c}{\omega^4 + \omega^2(0.1452\omega_p^2\xi^2 - \omega_c^2) - 0.006\,587\omega_p^4\xi^4}, \tag{7.22b}$$

$$\chi_{yy}^{(e)}(\vec{k}\omega) = -\frac{\omega_p^2 a_0}{2\pi}\frac{\omega^2 - \omega_p^2(-0.181\,48\xi_x^2 + 0.36\,297\xi_y^2)}{\omega^4 + \omega^2(0.1452\omega_p^2\xi^2 - \omega_c^2) - 0.006\,587\omega_p^4\xi^4}, \tag{7.22c}$$

where we have defined

$$\xi_x = a_0 k_x, \quad \xi_y = a_0 k_y. \tag{7.23}$$

We conclude this section by pointing out that if we substitute the sum of Eqs. (5.9) and (5.21) into Eq. (7.4), we obtain for the frequencies of the normal modes of vibration of the hexagonal Wigner crystal, in the long-wavelength limit and in the presence of the magnetic field (7.1),

$$\omega_1^2(\vec{q}) = \omega_c^2 + \omega_p^2(a_0 q) - \omega_p^2(0.145\,186)(a_0 q)^2 - (\omega_p^4/\omega_c^2)(0.036\,296\,7)(a_0 q)^3 + O(q^4), \tag{7.23a}$$

$$\omega_2^2(\vec{q}) = (\omega_p^4/\omega_c^2)(0.036\,296\,7)(a_0 q)^3 + O(q^4). \tag{7.23b}$$

On comparing these results with the corresponding ones obtained in the absence of the magnetic field and given by Eqs. (5.24), we see that the frequencies are still isotropic to this order in q. The principal effects of the magnetic field are the raising of the frequency of the higher-frequency longitudinal branch so that it tends to the nonzero limit ω_c as $q \to 0$, and the replacement of the linear dependence on q of the frequency of the lower frequency, transverse branch by a $q^{3/2}$ dependence. These results are in agreement with those recently obtained by Fukuyama.[17]

VIII. PLASMA OSCILLATIONS OF A TWO-DIMENSIONAL WIGNER CRYSTAL

The results of Sec. VII enable us to obtain the dispersion relation for the plasma oscillations of a two-dimensional Wigner crystal. The necessary theory has been worked out by Chiu and Quinn,[8] who assume that a two-dimensional electron gas occupies the plane $z = 0$ in a medium whose dielectric constant is ϵ_0. A constant magnetic field normal to this plane is present. They look for solutions of Maxwell's equations for an electromagnetic field which propagates in the y direction and whose amplitude decays exponentially with increasing distance from the plane $z = 0$. They find that such a solution exists provided that the following dispersion relation is satisfied:

$$\left(\chi_{xx}^{(e)}(\vec{k}\omega) - \frac{\beta c^2}{2\pi\omega^2}\right)\left(\chi_{yy}^{(e)}(\vec{k}\omega) + \frac{\epsilon_0}{2\pi\beta}\right) - \chi_{xy}^{(e)}(\vec{k}\omega)\chi_{yx}^{(e)}(\vec{k}\omega) = 0. \tag{8.1}$$

In this equation, $\vec{k} = (0, k_y)$ and

$$\beta^2 = k_y^2 - \epsilon_0\omega^2/c^2 > 0, \tag{8.2}$$

where c is the speed of light.

In the case that there is no external magnetic field, Eq. (8.1) reduces to the pair of equations

$$\frac{\omega_p^2 a_0}{2\pi}\frac{1}{0.036\,297\omega_p^2\xi^2 - \omega^2} = \frac{c^2}{2\pi a_0\omega^2}\left(\xi^2 - \epsilon_0 a_0^2\frac{\omega^2}{c^2}\right)^{1/2}, \tag{8.3a}$$

$$\frac{\omega_p^2 a_0}{2\pi}\frac{1}{0.18148\omega_p^2\xi^2 + \omega^2} = \frac{\epsilon_0 a_0}{2\pi}\left(\xi^2 - \epsilon_0 a_0^2\frac{\omega^2}{c^2}\right)^{-1/2}, \tag{8.3b}$$

where we have used the results given by Eqs. (7.22) for the elements of the dielectric susceptibility tensor, and have set $a_0 k_y \equiv \xi$.

Equation (8.3b) can be solved analytically, with the result that $\Omega \equiv \omega/\omega_p$ is given by

$$\Omega^2 = \frac{1}{2}\left\{-\left(\frac{\lambda^2}{\epsilon_0} + 0.362\,96\xi^2\right) + \left[\frac{\lambda^4}{\epsilon_0^2} + \left(0.725\,92\frac{\lambda^2}{\epsilon_0} + \frac{4}{\epsilon_0^2}\right)\xi^2\right]^{1/2}\right\}, \tag{8.4}$$

where for convenience we have set $\lambda = a_0\omega_p/c$. This dispersion curve is plotted in Fig. 3, as the

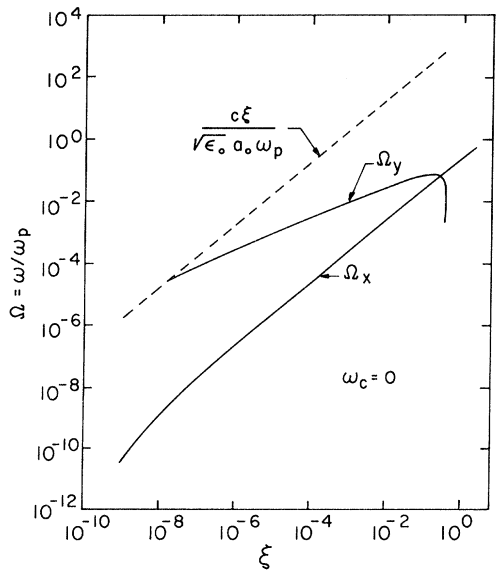

FIG. 3. Dispersion curves for the high (Ω_y) and low (Ω_x) frequency branches of the dispersion relation for the plasma oscillations of a two-dimensional hexagonal Wigner crystal imbedded in a dielectric medium whose dielectric constant is $\epsilon_0 = 16$. These curves are computed for zero external magnetic field. The curve labeled Ω_x is the solution of Eq. (8.3a); the curve labeled Ω_y is the solution of Eq. (8.3b).

curve labeled Ω_y, because it is the solution of the equation $\chi^{(e)}_{yy}(\vec{k}\omega) + \epsilon_0/2\pi\beta = 0$, with $\omega_c = 0$. The following values of the parameters have been used: $\epsilon_0 = 16$, $a_0 = 1000$ Å, $m^* = m_e$, where m_e is the electronic mass. With these values of the parameters $\omega_p = 4.826 \times 10^{10}$ rad/sec, and $\lambda = 1.4297 \times 10^{-4}$. In the long-wavelength limit this curve is asymptotic to the light line, $\Omega = \xi/\epsilon_0^{1/2}\lambda$ $(\omega = ck_y/\epsilon_0^{1/2})$.

Three comments should be made about the dispersion curve given by Eq. (8.4) and plotted as the curve Ω_y in Fig. 3. The first is that it is the analog of the result obtained for a two-dimensional electron gas by Chiu and Quinn[8] in the absence of an external, perpendicular magnetic field, in the sense that the only solution of Eq. (8.1) for $\omega_c = 0$ they found was the solution of the equation $\chi^{(e)}_{yy}(\vec{k}\omega) + \epsilon_0/2\pi\beta = 0$. The second is that the bending over of this curve for $\xi \approx 0.35$ is due to spatial dispersion, i.e., to the $\vec{k}$ dependence of the susceptibility $\chi^{(e)}_{yy}(\vec{k}\omega)$. Indeed, if the $\vec{k}$ dependence of $\chi^{(e)}_{yy}(\vec{k}\omega)$ is neglected, the solution of the equation $\chi^{(e)}_{yy}(\vec{k}\omega) + \epsilon_0/2\pi\beta = 0$ is

$$\Omega^2 = \tfrac{1}{2}[-\lambda^2/\epsilon_0 + (1/\epsilon_0)(\lambda^4 + 4\xi^2)^{1/2}], \tag{8.5}$$

a monotonically increasing function of ξ. Finally, the fact that this curve bends over so sharply that Ω^2 goes to zero at $\xi \approx 0.35$ is due to the large value of the background dielectric constant ϵ_0 assumed in these calculations. Indeed, we have carried out calculations of this dispersion curve for smaller values of ϵ_0, e.g., 2, and find that Ω^2 remains positive for values of ξ out to the Brillouin zone boundary.[18] In this regard it should be kept in mind that because we have used only the leading term in the small ξ expansion of the matrix elements $\bar{C}_{\alpha\beta}(\vec{k})$ entering the definition of $\chi^{(e)}_{\alpha\beta}(\vec{k}\omega)$, the dispersion curves we present are probably not reliable for values of ξ much larger than a few tenths.

Equation (8.3a) is not readily solved analytically. We have therefore solved it numerically for the values of the parameters given above. The result is also plotted in Fig. 3, as the curve labeled Ω_x, because it is the solution of the equation $\chi^{(e)}_{xx}(\vec{k}\omega) - \beta c^2/2\pi\omega^2 = 0$, with $\omega_c = 0$. In the limit of small ξ, it has the form

$$\Omega^2 \cong [0.036\,297/(\lambda^2 + \xi)]\xi^3. \tag{8.6}$$

It should be pointed out that the equation $\chi^{(e)}_{xx}(\vec{k}\omega) - \beta c^2/2\pi\omega^2 = 0$ has a solution for $\omega_c = 0$ in the present case only because of spatial dispersion. If the ξ dependence of the left-hand side of Eq. (8.3a) were neglected, this equation would have no solution.

In the presence of a magnetic field it is necessary to solve Eq. (8.1) numerically. We have carried out these calculations for $\omega_c = 0.1\omega_p$, $\omega_c = \omega_p$, and $\omega_c = 5\omega_p$, corresponding to magnetic fields of 274, 2744, and 13 718 G, respectively. In the presence of the magnetic field the dispersion curves change markedly from what they are in the absence of the field. The curve we have labeled Ω_x in Fig. 3 develops a gap, and now intersects the light line at a frequency close to $\omega_c(\Omega = \omega_c/\omega_p)$, instead of tending to zero with vanishing ξ. This branch is depicted for the three different values of ω_c in Fig. 4. [Strictly speaking, it is perhaps incorrect to refer to this branch of the plasma dispersion curve as the Ω_x branch, since in the presence of the external magnetic field it is a solution of the entire dispersion relation (8.1), rather than a zero of the first factor on the left-hand side of this equation. However, for very small ω_c, the effect of the last term on the left-hand side of Eq. (8.1) on the solutions of that equation is negligible in first approximation, so that even in the presence of an external magnetic field the dispersion curves are given by the zeros of each of the first two factors in this limit. This is the basis for our labeling of the solutions in the presence of the external field. In our work, however, the entire dispersion relation (8.1) was solved for nonzero ω_c to obtain the curves shown in Figs. 4–6.] The dispersion

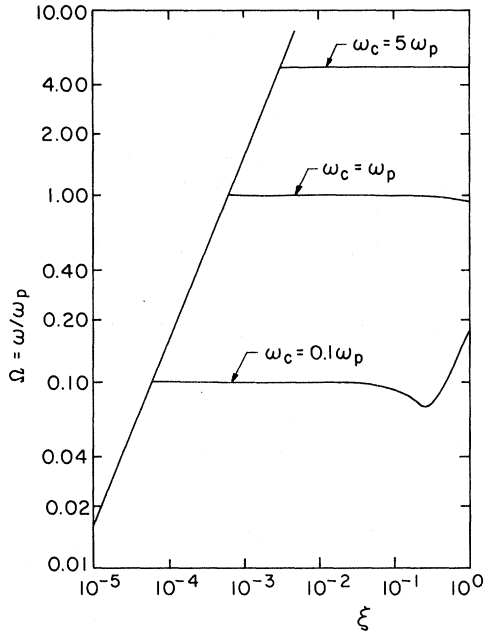

FIG. 4. Form the dispersion curve Ω_x of Fig. 3 takes in the presence of a static external magnetic field directed perpendicularly to the two-dimensional Wigner crystal.

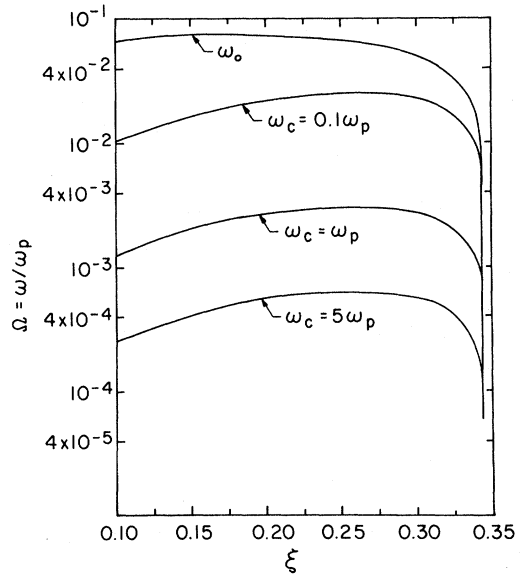

FIG. 6. Enlarged portion of Fig. 5 showing the magnetic field dependence of the lower frequency branch of the Ω_y dispersion curve for values of ξ close the critical value at which the dispersion curve goes to zero.

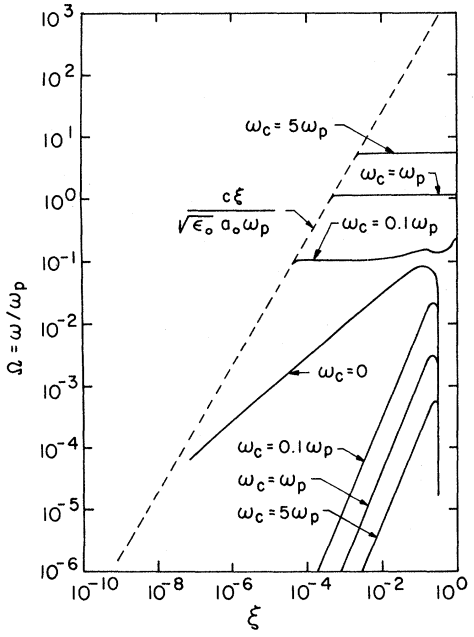

FIG. 5. Form the dispersion curve Ω_y of Fig. 3 takes in the presence of a static external magnetic field directed perpendicularly to the two-dimensional Wigner crystal.

curves shown in Fig. 4 are virtually independent of ξ in the range $0 < \xi \lesssim 1$, and have values close to the limiting value of ω_c over this entire range of ξ. This is the more pronounced the larger ω_c is. It is due to the fact that the terms $\omega^4 - \omega^2\omega_c^2$ dominate the others in the denominator of $\chi_{xx}^{(e)}(\vec{k}\omega)$ in the range of ξ considered, with the numerator never changing sign in this range.

The curve labeled Ω_y in Fig. 3 splits into two branches in the presence of an external magnetic field. This is shown in Fig. 5, for three different values of ω_c. The lower frequency branch can be thought of as the Ω_y branch of Fig. 3, depressed in frequency by the external magnetic field. For nonzero ω_c it bends over and goes to zero at the same value of ξ as in the case of no external magnetic field. This critical value of ξ is determined by the condition that $\chi_{yy}^{(e)}(\vec{k}\omega)$ be larger than $\epsilon_0/2\pi\beta$ at $\omega = 0$, and is independent of ω_c. The behavior of the lower-frequency branch as a function of ξ in the vicinity of this critical value of ξ is shown enlarged in Fig. 6, for three values of ω_c.

The higher frequency branch which develops in the Ω_y dispersion curve for nonzero ω_c resembles the curve Ω_x goes into in the presence of an external magnetic field. It also intersects the light line at a frequency close to ω_c, but lies slightly above the Ω_x curve. It is largely dispersionless, particularly for values of $\omega_c \gtrsim \omega_p$. It has the same origin as that of the gap that develops in the Ω_x

branch for nonzero ω_c, the fact that the denominator of $\chi_{yy}^{(e)}(\vec{k}\omega)$ is dominated by the terms $\omega^4 - \omega^2\omega_c^2$. However, the fact that there is a second branch in this case is due to the fact that the numerator of $\chi_{yy}^{(e)}(\vec{k}\omega)$ goes through zero at $\Omega = 0.19\xi$, in addition to the denominator changing sign at $\omega \approx \omega_c$, which affords the possibility of the factor $\chi_{yy}^{(e)}(\vec{k}\omega) + \epsilon_0/2\pi\beta$ vanishing for two values of ω for each value of ξ. The actual root is modified slightly by the presence of the last term on the left-hand side of Eq. (8.1), but this does not alter the qualitative explanation of the existence of two roots in this case.

IX. CONCLUSIONS

In this paper we have studied several static and dynamic properties of a two-dimensional Wigner crystal. By calculating the static ground-state energy for each of the two-dimensional Bravais lattices we have determined that the hexagonal lattice has the lowest energy of all structures of this type.

We have obtained the phonon dispersion curves along the symmetry directions in the two-dimensional Brillouin zone for the hexagonal crystal. In contrast with the dispersion curves for a three-dimensional Wigner Bravais crystal, in which the frequency of the longitudinal branch tends to a nonzero limiting value with vanishing wave vector, the dispersion curves for both branches of the spectrum of a two-dimensional Wigner Bravais crystal vanish with vanishing wave vector, the longitudinal branch as $q^{1/2}$, the transverse branch as q.[3,5] Our results, in the case of a hexagonal crystal are qualitatively similar to those of Platzman and Fukuyama[6] for the same crystal, but there are some quantitative differences between them. These may be due to the fact that these authors calculated the elements of the dynamical matrix by evaluating the slowly convergent sums in Eq. (3.6) by direct summation over the sites of the direct lattice, rather than by first transforming them into rapidly convergent expressions as we have done here. As a result, numerical inaccuracies may have entered the results obtained by Platzman and Fukuyama due to the use of poorly converged values for the elements of the dynamical matrix. We also find that the dispersion curve for the transverse branch along the direction $(q_x, 0)$ exhibits an anomalous upward curvature at about half the distance to the Brillouin-zone boundary, a feature which had not been noted in previous work.[5,6]

In contrast with the results of earlier calculations[5] we have also found that the square lattice is unstable in the long-wavelength limit.

The results for the normal-mode frequencies of the hexagonal crystal have been used to obtain the zero-point energy of the crystal, and the low-temperature specific heat, as a representative of the vibrational contribution to the thermodynamic properties of such a two-dimensional Wigner crystal. The latter property possesses the proportionality to the square of the absolute temperature, characteristic of the low-temperature specific heat of two-dimensional vibrating lattices.

Finally, we have studied the response of a two-dimensional Wigner crystal to a macroscopic electric field in the presence of a static, external magnetic field, and have obtained in this way the dielectric susceptibility of the crystal as a function of frequency and wave vector. The general expressions obtained have been evaluated in the long-wavelength limit for the hexagonal crystal, and the result used to obtain the dispersion relation for the plasma oscillations of the two-dimensional Wigner crystal embedded in a three-dimensional dielectric medium in the presence of an external magnetic field. The dispersion curves obtained differ qualitatively from those obtained for a two-dimensional electron gas by Chiu and Quinn[8] in possessing two branches, whose frequencies vanish with vanishing wave vector (in zero external magnetic field). The existence of these two branches may well be the single most characteristic feature of the two-dimensional Wigner crystal in comparing it with a two-dimensional electron gas. In the presence of an external magnetic field these dispersion curves are shifted, and new branches appear, which have no counterpart in the zero-field case, and which have no obvious counterpart in the dispersion curve for the plasma oscillations of a two-dimensional electron gas.[8] Observation of these features in the dispersion curves for a two-dimensional Wigner crystal would provide striking evidence of the crystallinity of the system.

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