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## Excitation spectrum of a two-dimensional Wigner lattice

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We propose a spectroscopic method to determine the existence of an electronic Wigner lattice at a given electron density  $n$ . We derive the “perpendicular” excited states of the two-dimensional Wigner lattice on a dielectric layer with a metallic substrate, and compare them with the corresponding excited states of the two-dimensional electron gas at the same electron densities. The transitions from the ground to the first excited state are studied in detail and we have found a significant difference between the lattice and the gas excitation energies for  $n \gtrsim 10^8 \text{ cm}^{-2}$ . In that sense, the spectroscopy of electronic transitions can prove the existence of a Wigner lattice and a rapid change in the excitation spectrum can serve for determination of the lattice melting temperature. A linear Stark effect in the case of a Wigner lattice is also analyzed.

### I. INTRODUCTION

The two-dimensional (2D) electron gas and its crystallization into a regular lattice at low electron densities has been extensively investigated since the electron lattice was predicted by Wigner almost 60 years ago.<sup>1</sup> However, an experimental detection of a Wigner lattice was a tedious task and it was found for 2D electrons on a liquid He surface by detecting a change in the microwave absorption due to the excitation of coupled plasmon-rippion modes parallel to the He surface.<sup>2</sup> Here we wish to present the possibility of another more direct way, based on the microwave absorption due to the perpendicular excitation of electrons in the lattice. A similar experiment was already performed<sup>3</sup> but at very low electron densities ( $n \lesssim 10^7 \text{ cm}^{-2}$ ), where the electron energy is mainly determined by the image potential of the substrate (liquid helium). In that case the electron-electron interaction is quite negligible, so that the 2D electron gas and the 2D Wigner lattice will have practically the same excitation spectra [see Fig. 2(a)].

At higher electron densities ( $n > 10^8 \text{ cm}^{-2}$ ) the electron-electron interaction begins to dominate over the image potential. In that case the calculation should give the different excitation spectra for electrons in the gas and crystal phases, and the analysis of experimental data could determine the phase for a given 2D electron density. Here, by 2D electrons we assume a quasi-2D electron system with perpendicular delocalization of an electron wave function.

The excitation spectrum in the 2D gas phase was already calculated for a wide range of electron densities.<sup>4</sup> In this paper we wish to calculate the excitation spectrum of the 2D Wigner lattice. Recent numerical calculations<sup>5</sup> indicate that the 2D Wigner lattice should exist for  $n \lesssim 8 \times 10^{12} \text{ cm}^{-2}$  (in the  $T \rightarrow 0$  limit) so we expect that our theory will correctly describe the excitation spectra of 2D electrons in this density range.

In the present paper we shall follow the theory developed in our previous papers,<sup>6–8</sup> where we have derived the ground-state energy of a 2D Wigner lattice on a dielectric layer with a metallic substrate. Within the same formalism in Sec. II we calculate the energies of excited states and thus determine the excitation spectra of a lattice. In Sec. III we give a simple theory of a 2D electron gas at low electron densities in order to compare the lattice and the gas-phase-excitation spectra. The results are discussed in Sec. IV. In the Appendix we derive explicit equations for the first excited state of a 2D Wigner lattice.

### II. FORMULATION OF THE PROBLEM

In order to determine the energies of excited states of the 2D Wigner lattice, we shall perform calculations similar to those for the ground-state energy in Refs. 6–8. The model Hamiltonian for a 2D electron system on a dielectric layer of thickness  $d$ , deposited on a (semi-infinite) metallic substrate is

$$H = \sum_i K_i + \sum_i W^{\text{im}}(z_i) + \frac{1}{2} \sum_{j \neq i} W^{\text{ee}}(\rho_{ij}; z_i, z_j). \quad (1)$$

Here,  $K$ ,  $W^{\text{im}}$ , and  $W^{\text{ee}}$  denote kinetic energy, image potential, and electron-electron interaction, respectively, and  $(z_i, z_j)$  are the perpendicular distances (with respect to the dielectric surface) of the two electrons at a lateral distance  $\rho_{ij}$ . All three terms in (1) are discussed in detail in Refs. 7 and 8.

#### A. Electron wave function in a Wigner lattice

The wave function  $\psi(\mathbf{r})$  of 2D electrons is approximated by a product of a lateral  $v(\rho)$  and a perpendicular  $u(z)$  part:<sup>6</sup>

$$\psi_l(\mathbf{r}) = v(\rho)u_l(z). \quad (2)$$

Here,  $\mathbf{r}=(\rho, z)$  denotes all coordinates of the system and  $l=0$  stands for the ‘‘perpendicular’’ ground state and  $l \geq 1$  for the  $l$ th excited state.

The excited perpendicular states of a 2D Wigner lattice correspond to a temperature above 6 K (Ref. 3) and the lattice exists typically below 2 K,<sup>2</sup> where we can assume that all electrons are in their perpendicular ground states. In the experiment, the perpendicular excitation is caused by a weak external electric field.<sup>3</sup> Since only a small fraction of electrons is excited, we can assume that an excited electron is surrounded by other electrons in the perpendicular ground state. In that sense, the perpendicular wave function takes the form of the Hartree approximation

$$u_l(z) = u_l(z_l) \prod_{j \neq l} u_0(z_j), \quad (3)$$

and  $u_l(z_l)$  are the one-particle variational wave functions. Now we define one-particle perpendicular Hartree energies as follows:

$$E_l = \langle K \rangle_l + \langle W^{\text{im}} \rangle_l + \langle W^{\text{ee}} \rangle_{0l}, \quad (4)$$

$$\langle K \rangle_l = \int dz u_l^*(z) \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \right] u_l(z), \quad (5a)$$

$$\langle W^{\text{im}} \rangle_l = \int dz |u_l(z)|^2 W^{\text{im}}(z), \quad (5b)$$

$$\langle W^{\text{ee}} \rangle_{0l} = \sum_{j \neq 0} \langle W^{\text{ee}}(\rho_j^0) \rangle_{0l}, \quad (5c)$$

$$\langle W^{\text{ee}}(\rho) \rangle_{0l} = \int dz \int dz' |u_0(z)|^2 |u_l(z')|^2 W^{\text{ee}}(\rho; z, z'). \quad (5d)$$

The functions  $u_l(z)$  are usually chosen to fit the perpendicular Schrödinger equation with the image potential  $W^{\text{im}}(z)$ . In this paper we shall study the lowest  $0 \rightarrow 1$  transition. The corresponding wave functions in the ‘‘hydrogenic’’ approximation<sup>3,6</sup> are

$$u_0(z) = A 2az e^{-az}, \quad (6a)$$

$$u_1(z) = B 2az(1 - baz) e^{-\beta az}. \quad (6b)$$

The orthonormality condition gives

$$A = \sqrt{\alpha}, \quad B = \frac{3\alpha b^5}{(\beta^2 - \beta + 1)}, \quad b = \frac{1}{3}(\beta + 1), \quad (7)$$

and only two independent variational parameters ( $\alpha, \beta$ ) remain. They are calculated by minimizing the functions  $E_0(\alpha)$  and  $E_1(\beta)$ . Although the Hartree approximation is not expected to give exact ground-state energy,<sup>6,7</sup> we expect it to give the correct perpendicular excitation spectrum  $E_{0l} = E_l - E_0$  of a 2D Wigner lattice.

In calculating the lattice potential (5c) we have assumed that all electrons acting on an electron at  $\rho_0^0=0$  are in their regular positions  $\rho_j^0$ . This approximation is justified in Ref. 6, where we have shown that the lateral lattice dynamics has negligible influence on the perpendicular wave function. This holds true at low temperatures ( $T \leq 2$  K) and at low electron densities ( $n \lesssim 10^{12}$  cm<sup>-2</sup>), where electrons remain well separated.

Both criteria are fulfilled in a real experimental situa-

tion.<sup>2</sup> For the same reason we shall neglect electron relaxation, which occurs because the surrounding electrons feel different potential when the  $\rho_0^0=0$  electron is excited from the ground state. However, for the first excited state (and a few higher states) the charge density  $e|u_l(z)|^2$  has almost the same effect on the surrounding electrons as  $e|u_0(z)|^2$ , providing that the electron density is not too high ( $n \lesssim 10^{12}$  cm<sup>-2</sup> for  $l=1$ ).

### B. Average interaction between electrons in a Wigner lattice

As discussed in Ref. 8, the lattice potential  $\langle W^{\text{ee}} \rangle_{0l}$  also contains the  $\mathbf{k}=0$  component, i.e., the average electron-electron interaction

$$\langle W_0^{\text{ee}} \rangle_{0l} = \frac{1}{S} \int d\rho \langle W^{\text{ee}}(\rho) \rangle_{0l}, \quad (8)$$

and  $S=1/n$  is the average area per electron. After averaging, this term can be divided into two parts,<sup>8</sup>

$$\langle W_0^{\text{ee}} \rangle_{0l} = 2\pi e^2 n \left[ \left[ \frac{1-\eta}{1+\eta} \right] 2d + \int dz |u_l(z)|^2 \langle W(z) \rangle_0 \right], \quad (9a)$$

$$\langle W(z) \rangle_0 = \int dz' |u_0(z')|^2 [(z+z') - |z-z'|]. \quad (9b)$$

Here,  $\eta=(\epsilon-1)/(\epsilon+1)$ , and  $\epsilon$  is the dielectric constant of the substrate.

The first term in the brackets in (9a) obviously diverges for  $d \rightarrow \infty$ . Since this term is the same for all energy levels  $l=0, 1, 2, \dots$ , this divergency is exactly canceled in the calculation of the electronic excitation spectra.

### III. ELECTRON STATES IN A 2D GAS

Here we calculate the excitation spectra of a 2D electron gas for the same densities ( $n \lesssim 10^{12}$  cm<sup>-2</sup>) within the local-density approximation. Assuming translational invariance along the  $\rho$  direction, the perpendicular Kohn-Sham equation<sup>9,10</sup> for the  $l$ th excited state of a 2D electron gas takes the form<sup>4,11-13</sup>

$$[K(z) + W^{\text{im}}(z) + \phi(z) + V^{\text{xc}}(z)] u_l^0(z) = E_l^0 u_l^0(z). \quad (10)$$

The first two terms in the brackets were already described,  $V^{\text{xc}}(z)$  is the local exchange-correlation potential, and  $\phi(z)$  is the electrostatic potential due to the (average) electron density

$$n(z) = \sum_j n_j |u_j^0(z)|^2. \quad (11)$$

Here,  $n_j$  is the density of occupied states in the  $j$ th perpendicular subband.

The potential  $\phi(z)$  satisfies the Poisson equation with the density  $n(z)$ , so we can write it in the integral form

$$\begin{aligned} \phi(z) &= \int d^3 r' n(z') W^{\text{ee}}(\rho; z, z') \\ &= 2\pi e^2 \eta \left[ \left[ \frac{1-\eta}{1+\eta} \right] 2d + \sum_j n_j \langle w(z) \rangle_j \right], \end{aligned} \quad (12)$$

$$\langle w(z) \rangle_j = \int dz' |u_j^0(z')|^2 [(z+z') - |z-z'|]. \quad (13)$$

Obviously,  $\phi(z)$  represents the  $\mathbf{k}=0$  component of the electrostatic potential  $\phi(\mathbf{r})$ . As in the case of  $\langle W_0^{ee} \rangle$ , it contains the term that diverges in the  $d \rightarrow \infty$  limit but which is exactly canceled in the calculation of the excitation spectra of a 2D electron gas.

At low densities, the Fermi energy of a 2D electron gas lies well below the first excited perpendicular state  $E_{1,3,4}^0$ . Therefore, at low temperatures we can assume that all electrons are in their perpendicular ground state  $E_0^0$ . The electron density is then approximated by

$$n(z) \approx n |u_0^0(z)|^2. \quad (14)$$

Although Eq. (10) should be solved self-consistently, the approximation (14) enables us to solve it using the same variational method as in the case of a Wigner lattice. Assuming that the image potential plays an important role, we can take even the same variational hydrogenic wave functions  $u_l^0(z) = u_l(z)$  as in the crystal phase. All those assumptions are not essential, but they will give us a closed relation between the gas and the crystal phase of 2D electrons.

In that sense, we can write Eq. (10) in the form

$$E_l^0 = \langle K \rangle_l + \langle W^{\text{im}} \rangle_l + \langle W_0^{ee} \rangle_{0l} + \langle V^{\text{xc}} \rangle_{0l}. \quad (15)$$

Here,  $\langle V^{\text{xc}} \rangle_{0l}$  is the average exchange-correlation potential for an electron in the  $l$ th excited state, assuming that all other electrons are in their ground states. All other terms in Eq. (15) have the same form as in the case of a Wigner lattice. Comparison between Eqs. (4) and (15) shows clearly that the attractive  $k > 0$  components of the lattice potential  $W^{ee}$  in a Wigner lattice are replaced by the attractive exchange-correlation potential  $V^{\text{xc}}$  of an electron gas.

The main problem in the Kohn-Sham approach is in deriving the effective potential  $V^{\text{xc}}(z)$ . As we have pointed out, Eq. (10) was already solved self-consistently,<sup>4</sup> with the Hedin-Lundqvist<sup>14</sup> form for  $V^{\text{xc}}(z)$ . This simple form was originally derived for a 3D electron gas but can also be successfully applied to the 2D electron gas, as described in detail, e.g., in Ref. 12. Although more refined forms of  $V^{\text{xc}}(z)$  were also proposed,<sup>11–13</sup> calculations have shown that  $V^{\text{xc}}(z)$  has an important influence on the ground-state energy of the 2D electron gas, but has little influence on the excitation spectrum at densities  $n \lesssim 10^{12} \text{ cm}^{-2}$ .<sup>4,12</sup> Also, the difference between the self-consistent and the variational approaches at those densities is expected to be small.<sup>15</sup> In that sense, we shall use the Hedin-Lundqvist form for  $V^{\text{xc}}(z)$  and perform the variational calculation to determine the excitation spectrum  $E_{0l}^0 = E_l^0 - E_0^0$  of the 2D electron gas from Eq. (15). If we assume the same effective mass for the ground and the  $l$ th excited states, the excitation spectrum  $E_{0l}^0$  will not depend upon the electron wave vector  $\mathbf{k}$ . We have checked that our results are in very good agreement with the self-consistent results presented in Ref. 4 [Fig. 2(a)]. The difference between the gas-phase curves at  $d=100 \text{ \AA}$  demonstrates the influence of the substrate that supports the He layer: we use the metallic substrate ( $|\epsilon| = \infty$ ), while the calculations in Ref. 4 were performed for sapphire ( $\epsilon = 19$ ).

#### IV. DISCUSSION OF ELECTRONIC EXCITATION SPECTRA

The  $0 \rightarrow 1$  transition of a 2D Wigner lattice is determined by the two parameters  $(\alpha, \beta)$ . Parameter  $\alpha$  and other relevant quantities concerning the ground state were analyzed in Ref. 8. The corresponding results for the first excited state are given in the Appendix.

Figure 1 shows parameter  $\beta$  as a function of a 2D hexagonal lattice parameter  $r_0$ . The hydrogenic value  $\beta=0.5$  is obtained in the limit  $r_0 \rightarrow \infty$ ,  $d \rightarrow \infty$ , where the variational wave functions (6) are exact solutions of the perpendicular Schrödinger equation. The deviation from that value at finite values of  $r_0$  and/or  $d$  is more pronounced in the case of He ( $\epsilon=1.057$ ) than in the Ar ( $\epsilon=1.66$ ) case because the influence of the image potential of the Ar substrate is much stronger.

The  $0 \rightarrow 1$  excitation energies of a Wigner lattice, which are supposed to exist at densities  $n < 8 \times 10^{12} \text{ cm}^{-2}$  in the  $T \rightarrow 0$  limit,<sup>5</sup> are shown in Fig. 2 as functions of electron density  $n$ . The  $0 \rightarrow 1$  excitation energies of a 2D electron gas are also shown to emphasize the differences between these two systems. The measurements of the  $0 \rightarrow 1$  transition at electron densities where these differences are significant ( $\gtrsim 1 \text{ meV}$  in Fig. 2) can lead to determination of the phase of 2D electrons for a given temperature. By changing the temperature, the phase transition should also be detected as the rapid change in the electronic excitation energy.

Significant difference between the crystal and gas phases is obtained at densities  $n \gtrsim 10^8 \text{ cm}^{-2}$  for the semi-infinite He substrate [Fig. 2(a)]. Early evidence of the Wigner lattice<sup>2</sup> was obtained exactly at these densities ( $10^8 \text{ cm}^{-2} < n < 10^9 \text{ cm}^{-2}$ ), so our theory can be experimentally verified.

For a thin He layer on a metallic substrate, or in the case of an Ar layer [Fig. 2(b)], a significant difference between the crystal and gas phases is obtained at higher

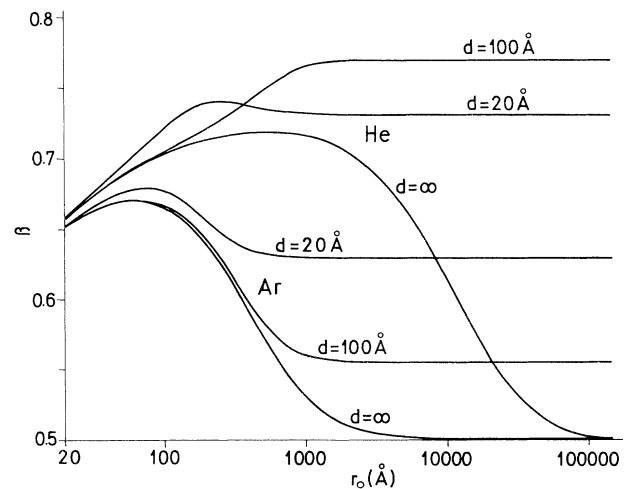


FIG. 1. Optimized values of the parameter  $\beta$  for the Wigner lattice for three different thicknesses  $d$  of He and Ar layers, as functions of the hexagonal lattice parameter  $r_0$ .

densities ( $n \gtrsim 10^9 \text{ cm}^{-2}$ ), due to the stronger image potential. However, this image potential also enables one to reach higher electron densities<sup>16,17</sup> so, again, the phase of the 2D electrons can be determined by measuring the  $0 \rightarrow 1$  transition.

Let us note that the parameters  $(\alpha, \beta)$  have larger values in the Wigner crystal than in the gas phase, which leads to stronger perpendicular localization of the crystal

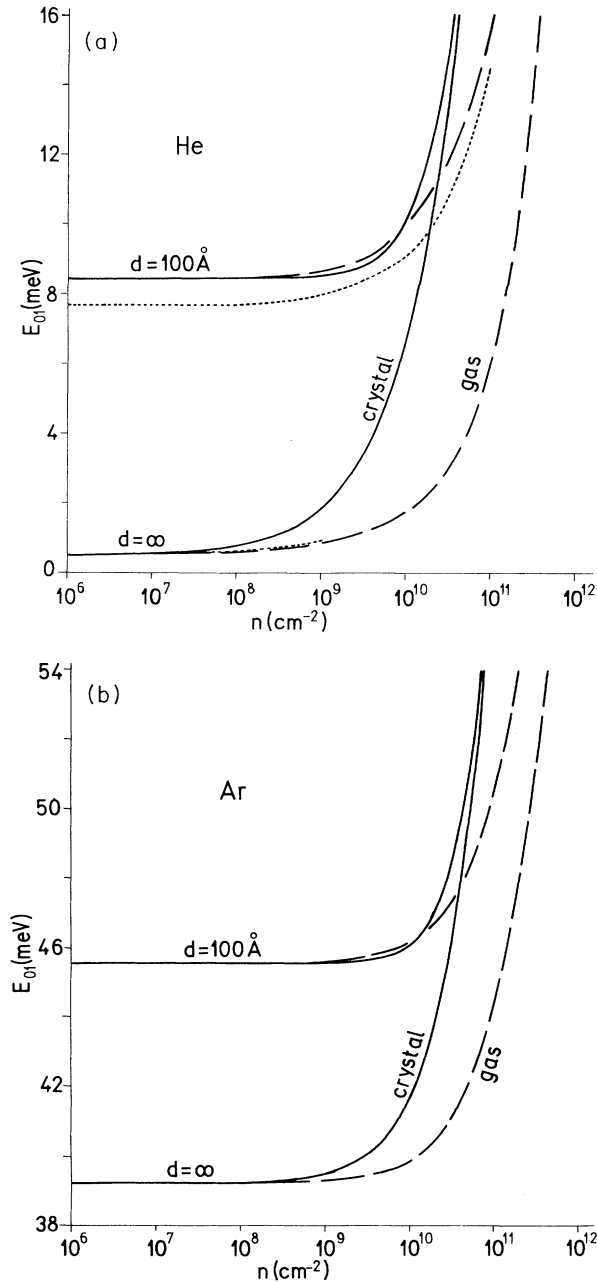


FIG. 2. Excitation energies  $E_{01} = E_1 - E_0$  of 2D electrons in the case of a crystal (full lines) and a gas (dashed lines) phase, as functions of electron density  $n$ . Two different thicknesses of (a) He and (b) Ar substrates are chosen. The dotted lines in (a)

wave function. This is particularly evident for parameter  $\beta$  at higher electron densities, which explains the difference in the  $0 \rightarrow 1$  transition energies between the crystal and gas phases.

#### A. Possible corrections to the model

It is necessary to point out the simplicity of our approach, which is based on the determination of the one-electron hydrogenic wave functions. Although some effects are neglected (e.g., the influence of anharmonicity on the electron-electron interaction in the Wigner lattice or the more precise determination of the exchange-correlation potential in the electron gas), they can, in principle, be calculated as a perturbation, using the hydrogenic wave functions  $u_l(z)$  with, eventually, the small change in the variational parameters  $(\alpha, \beta, \dots)$ . Here we shall give two examples.

##### 1. External electric field

An external constant electric field  $E$  is normally applied in the perpendicular direction in order to press the 2D electrons on the dielectric surface. In the Hartree approximation (3) the contribution of  $E$  to the excited state  $E_l$  (or  $E_l^0$ ) is simply given by

$$\langle W^E \rangle_l = eE \langle z \rangle_l, \quad (16)$$

$$\langle z \rangle_l = \int dz |u_l(z)|^2 z. \quad (17)$$

This “linear Stark effect” was already measured at very low electron densities ( $n \approx 10^5 \text{ cm}^{-2}$ ), i.e., in the ( $r_0 \rightarrow \infty$ ,  $d \rightarrow \infty$ ) limit.<sup>3</sup>

As pointed out in Ref. 4, the internal electric field caused by the image potential is usually much stronger than the pressing field. In that case, we can again use the variational functions (6) to determine the  $0 \rightarrow 1$  excitation energy.

Parameters  $\alpha$  and  $\beta$  for a 2D Wigner lattice as functions of external electric field  $E$  are shown in Fig. 3. Only the parameter  $\beta$  [Fig. 3(b)] for the He substrate at the ( $r_0 \rightarrow \infty$ ,  $d \rightarrow \infty$ ) limit is significantly affected by  $E$ . At higher electron densities (e.g.,  $r_0 = 1000 \text{ \AA}$ ,  $n \approx 10^{10} \text{ cm}^{-2}$ ) or for thinner dielectric layers (e.g.,  $d = 100 \text{ \AA}$ ),  $\beta$  remains almost independent of  $E$  because the electron-electron interaction and/or the image potential suppresses the influence of  $E$ . In the Ar case,  $\langle W^{\text{im}} \rangle$  is larger than  $\langle W^E \rangle$ , even in the  $d \rightarrow \infty$  limit. The same holds true for the gas phase.

This is again demonstrated in Fig. 4, where we have shown the excitation energy  $E_{01}$  of a Wigner lattice as a function of  $E$  for the He substrate. Obviously, the small change in  $E_{01}$  with  $E$  for both crystal and gas phases means that  $E_{01}$  is essentially determined by the  $(r_0, d)$  values. In that sense, the Stark effect is not a suitable method for the determination of the phase of 2D electrons.

##### 2. Electron penetration into the substrate

The influence of the penetration of electron density into the substrate was calculated in several ways, with al-

most the same result for the energy shift  $\Delta E_l$  of the  $l$ th energy level.<sup>18–20</sup> We shall use the perturbative treatment,<sup>18</sup> which connects  $\Delta E_l$  to the slope of the unperturbed wave function  $u_l(z)$  at the  $z=0$  dielectric surface:

$$\Delta E_l = \frac{\hbar^2}{2m} \left[ a - \left[ \frac{\hbar^2}{2mV_0} \right]^{1/2} \right] \left[ \frac{d}{dz} u_l(0) \right]^2. \quad (18)$$

Here,  $V_0$  is the potential barrier at the dielectric surface and  $\alpha$  is an adjustable parameter. With  $V_0=1$  eV and  $a=1.04$  Å, Eq. (18) gives almost a perfect fit the excita-

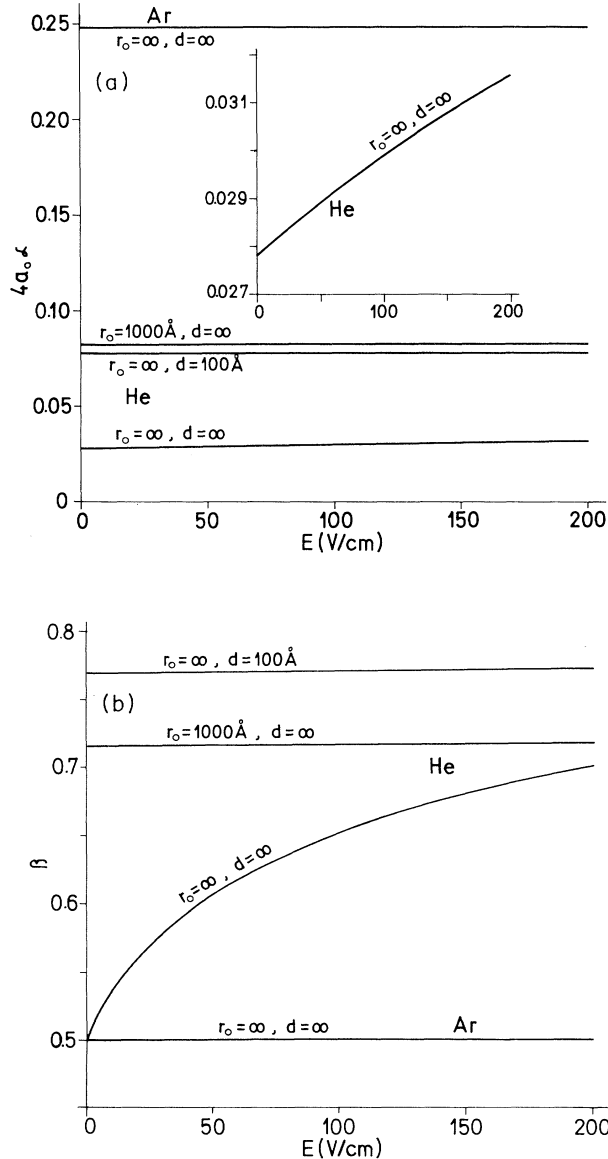


FIG. 3. Optimized values of (a)  $\alpha$  [in units  $(4a_0)^{-1}$ ,  $a_0$  is the Bohr radius] and (b)  $\beta$  for the Wigner lattice as functions of external electric field  $E$ . The inset of (a) shows the small change of  $\alpha$  even in the case of the He substrate in the  $(r_0 \rightarrow \infty, d \rightarrow \infty)$  limit. The Ar substrate gives in all cases almost constant values of both parameters  $(\alpha, \beta)$ .

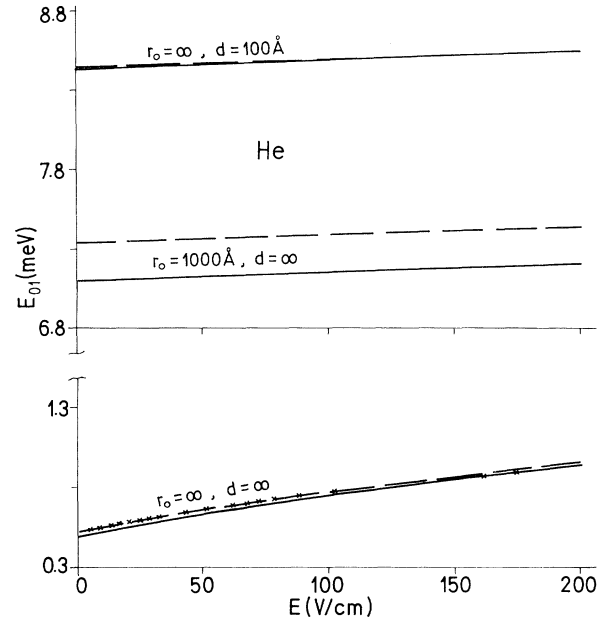


FIG. 4. Excitation energies  $E_{01}$  of the 2D Wigner lattice on the He layer, as functions of external electric field  $E$ . The correction due to electron penetration into the He surface is shown by dashed lines. The experimental values (Ref. 3) are shown by crosses.

tion spectrum of 2D electrons on a He substrate.<sup>3</sup> The influence of the shift (18) on the  $0 \rightarrow 1$  excitation energies is too small to be seen on the scale of Fig. 2, but we can see it on the scale of Fig. 4.

## V. CONCLUSIONS

In conclusion, we have derived the perpendicular excitation spectrum of a 2D electron Wigner lattice and analyzed the variation of the  $0 \rightarrow 1$  excitation energy as a function of electron density and a thickness and dielectric constant of the supporting dielectric layer. At electron densities  $n \lesssim 10^{12} \text{ cm}^{-2}$ , where possible corrections to the excitation spectrum are not significant, we expect our theory to give correct results, and this is exactly the density range at which a 2D Wigner lattice exists. Combined with the results for the excitation spectra of a 2D electron gas, our calculations can be used to determine the phase of 2D electrons in a wide density range ( $10^8 \text{ cm}^{-2} < n < 10^{12} \text{ cm}^{-2}$ ). Specifically, at these electron densities the rapid change in the excitation spectrum at the transition temperature can be used to detect the 2D Wigner phase transition.

## APPENDIX: THE FIRST EXCITED STATE VARIATIONAL DERIVATION

The kinetic energy operator

$$\mathbf{K} = -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} \quad (A1)$$

and the image potential<sup>8</sup>

$$W^{\text{im}}(z) = -\frac{1}{2}e^2 \int \mathbf{dk} D(k)e^{-2kz}, \quad (\text{A2})$$

$$D(k) = \frac{\eta + e^{-2kd}}{1 + \eta e^{-2kd}}, \quad \eta = \frac{\varepsilon - 1}{\varepsilon + 1},$$

are easily averaged using the function  $u_1(z)$  [Eq. (6b)] as follows:

$$\langle K \rangle_1 = \frac{e^2}{a_0} \frac{(\alpha a_0)^2 \beta^2}{6} \frac{(7\beta^2 - \beta + 1)}{(\beta^2 - \beta + 1)}, \quad (\text{A3})$$

$$\begin{aligned} \langle W^{\text{im}} \rangle_1 = & -\frac{3}{2} \frac{e^2}{a_0} \frac{\alpha a_0 \beta^5}{(\beta^2 - \beta + 1)} \\ & \times \int_0^\infty dx \frac{D(\alpha x)}{(\beta + x)^3} \left[ 1 - \left[ \frac{\beta + 1}{\beta + x} \right] \right. \\ & \left. + \frac{1}{3} \left[ \frac{\beta + 1}{\beta + x} \right]^2 \right]. \end{aligned} \quad (\text{A4})$$

The lattice potential  $\langle W^{\text{ee}} \rangle_{01}$  [Eq. 5(c)] is calculated by transferring the electron-electron interaction (5d) into the "x space"<sup>6</sup> as follows:

$$\langle W^{\text{ee}}(\rho) \rangle_{01} = e^2 \frac{2}{\sqrt{\pi}} \int_0^\infty dx e^{-\rho^2 x^2} f(x). \quad (\text{A5})$$

The function  $f(x)$  is now defined as

$$\begin{aligned} f(x) = & \int dz \int dz' |u_0(z)|^2 |u_1(z')|^2 \\ & \times \left[ e^{-(z-z')^2} \right. \\ & \left. - \sum_{n=-1}^\infty b_n e^{-[z+z'+2(n+1)d]^2 x^2} \right], \end{aligned} \quad (\text{A6})$$

$$b_{-1} = \eta; \quad b_n = (-)^n (1 - \eta^2)^n \eta^n, \quad n \geq 0.$$

If we write  $|u_1(z)|^2$  in a similar form as  $|u_0(z)|^2$  [Eq. (6)],

$$|u_1(z)|^2 = B^2 \left[ 1 + b \frac{\partial}{\partial \beta} + \frac{b^2}{4} \frac{\partial^2}{\partial \beta^2} \right] (2\alpha z)^2 e^{-2\alpha z \beta}, \quad (\text{A7})$$

we can calculate  $f(x)$  by a method similar to that given in the Appendix of Ref. 6. However, after taking the derivatives in (A7), the explicit result becomes lengthy and will not be given here. With the function  $f(x)$  defined by Eq. (A6) we can perform the summation in Eq. (5c) exactly as in Ref. 6.

The essential part of the average electron-electron interaction  $\langle W_0^{\text{ee}} \rangle_{01}$  in Eq. (9) is given by

$$\begin{aligned} & \int dz |u_1(z)|^2 \langle W(z) \rangle_0 \\ & = \frac{1}{\alpha} \left[ 3 - \left[ \frac{\beta}{\beta + 1} \right]^5 \frac{(3\beta^2 - 10\beta + 10)}{(\beta^2 - \beta + 1)} \right], \end{aligned} \quad (\text{A8})$$

while the average interaction (16) with the external electric field  $E$  becomes

$$\langle W^E \rangle_1 = eE \frac{1}{2\alpha\beta} \frac{(2\beta^2 - 2\beta + 5)}{(\beta^2 - \beta + 1)}. \quad (\text{A9})$$

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