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Lenac, Z.; Šunjić, Marijan

Permanent link / Trajna poveznica: https://urn.nsk.hr/urn:nbn:hr:217:874046

Download date / Datum preuzimanja: **2024-11-25**

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Hartree model of electrons in a two-dimensional Wigner lattice on a dielectric substrate

Z. Lenac
Pedagogical Faculty, YU-51000 Rijeka, Croatia, Yugoslavia

M. Šunjić
Department of Physics, University of Zagreb, P.O. Box 162, YU-41001 Zagreb, Croatia, Yugoslavia
(Received 17 May 1990; revised manuscript received 28 September 1990)

The wave functions and energies of electrons in a two-dimensional Wigner lattice above the surface of a dielectric (He, Ar) are determined in the Hartree approximation and compared with the classical result. The lattice sum is performed with the Ewald transformation, which is modified to include the effective electron-electron interaction in a rather general form. The electron binding energies are enhanced compared to the point-electron results due to electron delocalization perpendicular and parallel to a dielectric surface. The perpendicular delocalization is strongly correlated with the lateral electron interaction.

I. INTRODUCTION

It is well known that electrons above a liquid helium surface can form a (hexagonal) Wigner lattice at low temperatures and densities.[1,2] The phase diagram for this system was calculated[3] assuming strictly two-dimensional (2D) point electrons, and their Coulomb repulsion was calculated in the classical approximation. In fact, if we put a strictly 2D electron lattice on a flat dielectric surface, the electrostatic interaction of electrons with their image charges becomes infinite. To avoid this problem, the dielectric layer was usually treated simply as a vacuum layer ($\epsilon = 1$), which eventually separates the electron lattice from the metallic substrate.[4,5]

For 2D electrons moving freely along the dielectric surface, the electron distribution perpendicular to the surface was described as given by the hydrogenlike wave function[6-9] and the theory agreed very closely with the experimental results.[10] Recently, the energy of the few lowest electron levels was calculated in a self-consistent way.[11]

In our previous paper[12] we calculated phase diagrams for 2D electron lattice on a flat dielectric layer deposited on a metallic substrate, taking into account the perpendicular delocalization of electrons' wave functions and we showed how this modifies the Coulomb interaction. The wave functions were calculated in the attractive electrostatic potential of the metal and the dielectric assuming a strong repulsive potential at the surface due to the excitation gap in the rare-gas solid substrate.

This quantum-mechanical treatment of electrons immediately leads to the question of the self-consistency of the model—namely, the electron densities and their energies evaluated in the electrostatic substrate potential are expected to be modified due to the Coulomb repulsion of the 2D electron lattice.

In this paper we therefore analyze the properties of a two-dimensional electron Wigner lattice on a dielectric with an arbitrary dielectric constant, in a Hartree approximation. We minimize the Hartree Hamiltonian by taking into account simultaneously (i) the attractive electron interaction with the substrate (electron screening), and (ii) the repulsive interaction of each electron with all other electrons and their images.

The paper is organized as follows. In Sec. II, we formulate the problem and derive the appropriate Hartree Hamiltonian. In Sec. III we find the wave functions and energies of electrons in the ground state of a Wigner lattice in the Hartree approximation. The results are discussed in Sec. IV. The details of calculations regarding the lattice sums for a rather general shape of electron-electron potential are described in the Appendix.

II. FORMULATION OF THE PROBLEM

The electrons in a Wigner lattice on a dielectric substrate are localized at sites $\mathbf{r}_i \equiv (\boldsymbol{\rho}_i, z_i)$, and their Hartree Hamiltonian has the form

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

Here $K_i = -\hbar^2 \Delta_i / 2m$ is the kinetic energy operator; $W^{\text{im}}(z_i)$ is the electrostatic interaction (image potential) of the electron i, at distance z_i above the surface of the dielectric substrate. $W^{e-e}(\rho_{ij}; z_i, z_j)$ is the Coulomb interaction of the electron i (charge e) with all other electrons at lateral distances $\rho_{ij} = |\boldsymbol{\rho}_i - \boldsymbol{\rho}_j|$ from the electron i, and with all their images (lattice potential).

In deriving the image potential, we assume that the electrons cannot penetrate into the dielectric for energies in the region of the energy gap, as for He, Ar, Ne. In $\mathbf{k}$ space ($\mathbf{k}$ is a two-dimensional wave vector parallel to the surface) we can write[13]

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

where

$$D(\mathbf{k}, \omega) = \frac{\epsilon_s(\mathbf{k}, \omega) - 1}{\epsilon_s(\mathbf{k}, \omega) + 1}$$

and ϵ_s is the surface dielectric function,[13(a)] to be derived microscopically.

In the long-wavelength and low-frequency limit this reduces to the classical result:

$$D(k\to 0,\omega\to 0)=\beta, \quad \text{where } \beta=\frac{\epsilon-1}{\epsilon+1} \tag{3}$$

and ϵ is the static dielectric constant of the substrate. The image potential (2) now becomes

$$W^{\mathrm{im}}(z)=-\beta\frac{e^2}{4z} . \tag{4}$$

Screened static Coulomb interaction between two electrons at points $(\rho=0,z)$ and (ρ,z') can be written in the form

$$W^{e\text{-}e}(\rho;z,z')=\frac{A}{(2\pi)^2}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\boldsymbol{\rho}}W(k;z,z') , \tag{5}$$

where A is the dielectric surface (normalization) area and the Fourier components are [13(b),13(c)]

$$W^{e\text{-}e}(k;z,z')=\frac{(2\pi)^2}{A}\frac{e^2}{2\pi k}(e^{-k|z-z'|}$$
$$-D(k,\omega=0)e^{-k(z+z')}). \tag{6}$$

Here the first term is the direct and the second term is the induced (image) interaction. With the approximation (3) we find the well-known result in real space:

$$W^{e\text{-}e}(\rho;z,z')=e^2\left[\frac{1}{[(z-z')^2+\rho^2]^{1/2}}\right.$$
$$\left.-\frac{\beta}{[(z+z')^2+\rho^2]^{1/2}}\right] . $$

In the limit $k\to 0$, we find from (6)

$$W(k\to 0;z,z')=\frac{2\pi e^2}{A}\lim_{k\to 0}\left[\frac{1}{k}[1-D(k,0)]\right.$$
$$\left.+D(k,0)(z+z')-|z-z'|\right] . $$
$$\tag{7}$$

For a dielectric, with $D\to\beta$, the first term in the large parentheses diverges, because of the imperfect screening of electrons in the system. Only for $\beta\to 1$, i.e., metallic screening, the electrons are completely screened and the system can satisfy charge neutrality.

Generally, it is assumed that the lattice is stabilized by an external field arising, e.g., from the positive background,[14,2] which simulates the real experimental setup. The electron interaction with this external (macroscopic) field corresponds to the $k=0$ component of (6):

$$W_{\mathrm{ext}}(z,z')\equiv\frac{1}{A}\int d\rho\, W^{e\text{-}e}(\rho;z,z')$$
$$=W(k=0;z,z') . \tag{8}$$

This energy has to be subtracted in the calculation of the total electrostatic energy of the electron lattice.

In the Hartree approximation we neglect the exchange effects and treat the dynamics of the electron i in the mean field of all other electrons $j\neq i$. We shall show later that this approximation describes electrons in the Wigner lattice very well in their ground states, where they stay well localized at their lattice sites even at rather high densities. Moreover, the exchange energy was shown to be negligible even in the case of "free" 2D electrons.[11]

The electron wave function $\psi(\mathbf{r}_i)$ and energy E are given by

$$H_i\psi(\mathbf{r}_i)=E\psi(\mathbf{r}_i) , \tag{9}$$

and the mean field of all other electrons is described by their effective charge densities $e^2|\psi(\mathbf{r}_j)|^2$. The solution of an integrodifferential Hartree equation (9) is equivalent to finding variationally the extrema of the operator H_i. Therefore we shall search for the optimum trial wave function $\psi(\mathbf{r}_i)$ by minimizing the functional:

$$H_i\{\psi(\mathbf{r}_i)\}=\langle K\rangle+\langle W^{\mathrm{im}}\rangle+E_{\mathrm{pot}} , \tag{10}$$

where

$$\langle K\rangle=\int d\mathbf{r}_i\,\psi^*(\mathbf{r}_i)\left[-\frac{\hbar^2}{2m}\Delta_i\right]\psi(\mathbf{r}_i) , \tag{11a}$$

$$\langle W^{\mathrm{im}}\rangle=\int d\mathbf{r}_i|\psi(\mathbf{r}_i)|^2W^{\mathrm{im}}(z_i) , \tag{11b}$$

and E_{pot} is the effective (electron) lattice potential:

$$E_{\mathrm{pot}}=\langle W^{e\text{-}e}\rangle-\langle W^{e\text{-}e}(k=0)\rangle , \tag{11c}$$

$$\langle W^{e\text{-}e}\rangle=\sum_{j\neq i}\int\int d\mathbf{r}_i d\mathbf{r}_j|\psi(\mathbf{r}_i)|^2|\psi(\mathbf{r}_j)|^2W^{e\text{-}e}(\rho_{ij};z_i,z_j) . $$
$$\tag{11d}$$

III. DETERMINATION OF THE ELECTRON WAVE FUNCTION

We shall assume the trial electron wave function, appropriate for the ground state of the Wigner lattice, in the form

$$\psi(\mathbf{r}_i)=u(z_i)v(\boldsymbol{\rho}_i-\boldsymbol{\rho}_i^0) , \tag{12}$$

where

$$u(z_i)=2\alpha^{3/2}z_i e^{-\alpha z_i} , \tag{13a}$$

$$v(\boldsymbol{\rho}_i-\boldsymbol{\rho}_i^0)=\frac{1}{\sqrt{\pi}\sigma}e^{-1/2\left[\frac{\boldsymbol{\rho}_i-\boldsymbol{\rho}_i^0}{\sigma}\right]^2} , \tag{13b}$$

and $\boldsymbol{\rho}_i^0$ is the regular (equilibrium) lateral position of the ith electron in the lattice. The two parameters (α,σ) should be determined by minimizing the Hamiltonian (10).

Here we shall briefly argue why the wave function (12) can be factorized, and a more rigorous proof will be derived in the following sections, together with the form of these factors.

The first two terms K and W^{im} in the Hamiltonian (1) depend separately on ρ and z coordinates. We have analyzed the third term (lattice potential), assuming a small

displacement $\Delta\rho_i$ of the electron i from its equilibrium position:

$$\sum_{j\neq i} W^{e-e}(\rho_i^0 + \Delta\rho_i - \rho_j^0; z_i, z_j)$$

$$= \sum_{j\neq i} W^{e-e}(\rho_{ij}^0; z_i, z_j) + \gamma(z_i, z_j)(\Delta\rho_i)^2 + \cdots \ , \qquad (14)$$

and the harmonic constant γ can be put in the form

$$\gamma = -\frac{A}{4\pi} \sum_{j\neq i} \cos^2\beta_j \int_0^\infty dk\, k^3 J_0(k\rho_{ij}^0) W^{e-e}(k; z_i, z_j) \ .$$

Here β_j is the angle between ρ_{ij}^0 and $\Delta\rho_i$, and J_0 is the Bessel function. When we average the potential (14), and therefore $\gamma(z_i, z_j)$, over the z coordinates, e.g., with the functions $u(z)$, Eq. (13a), and perform the summation over at least four electron shells, we obtain (to within 1%) the same value for γ regardless of the choice of the parameter α in the functions $u(z)$ and regardless of the direction in the crystal.

In this way we have shown that the whole effective Hamiltonian can be assumed, in the harmonic approximation (14), to depend separately on ρ and z. This holds true for all realistic physical situations, i.e., for $\beta \lesssim 0.3$, $4\alpha a_0 \gtrsim \beta$, and $\Delta\rho_i \lesssim 0.3 r_0$ [which is the condition for the harmonic approximation (14)]. Here a_0 is the Bohr radius and r_0 is the lattice constant. Therefore an electron will feel the same harmonic potential in the ρ direction regardless of its perpendicular delocalization, i.e., the parameters α and σ should be almost independent.

The physical meaning of the two variational parameters is obvious: Parameter σ gives th lateral spread of the electron density, while the mean perpendicular position of the electron

$$\langle z \rangle = \frac{3}{2\alpha} \qquad (15a)$$

and its perpendicular width

$$\Delta z \equiv (\langle z^2 \rangle - \langle z \rangle^2)^{1/2} = \frac{\sqrt{3}}{2\alpha} \qquad (15b)$$

are determined by α.

The classical (point-electron) approximation is obtained for $\alpha \rightarrow \infty$, $\sigma \rightarrow 0$:

$$|u(z_i)|^2 \underset{\alpha\rightarrow\infty}{\longrightarrow} \delta(z_i) \ , \qquad (16a)$$

$$|v(\rho_i - \rho_i^0)|^2 \underset{\sigma\rightarrow 0}{\longrightarrow} \delta(\rho_i - \rho_i^0) \ . \qquad (16b)$$

Inserting (12) and (13) into (11) we find the mean kinetic energy and image potential:

$$\langle K \rangle = \frac{e^2}{2} a_0 (\alpha^2 + 1/\sigma^2) \ , \qquad (17a)$$

$$\langle W^{im} \rangle = -\beta\frac{e^2}{4}\alpha \ . \qquad (17b)$$

The $k=0$ component of (7), summed over all electrons, becomes

$$\langle W^{e-e}(k=0)\rangle = \frac{2\pi}{S}e^2 \lim_{k\rightarrow 0}\left[(1-\beta)\frac{1}{k} + (3\beta - \tfrac{15}{16})\frac{1}{\alpha}\right] .$$
$$(18)$$

Here $S \equiv A/\sum_j 1$ is the average area per electron. Now we have to determine the effective lattice potential E_{pot} (11c).

One can easily obtain the interaction between two electrons in direct or in Fourier space, but the summation converges extremely slowly due to the long range of the Coulomb interaction.

An analogous summation in the case of the two-dimensional classical (point-electron) Wigner lattice was performed by Bonsall and Maradudin,[14] who used the fast-convergent Ewald transformation appropriate for the $1/\rho$ potential. Peeters and Platzman[4,5] slightly modified this method in order to include the electron screening. We shall here adopt basically the same procedure, but for a more general form of the potential. Our approach can be applied to various problems and therefore we describe the detailed calculations in the Appendix.

Although the calculations do not depend upon the symmetry of the Wigner lattice, we shall perform (numerical) calculations for the hexagonal lattice, which turns out to be the most stable configuration.[5] In that case the relation between the direct r_0 and the reciprocal g_0 lattice vectors is

$$g_0 = 2\pi r_0/S, \quad S = \tfrac{1}{2}\sqrt{3}r_0^2 \ . \qquad (19)$$

A. Perpendicular delocalization of electron density

Here we shall briefly analyze the perpendicular spread of an electron wave function $u(z)$, neglecting the lateral spread of the electron density ($\sigma = 0$).

In the case of a single electron interacting with the substrate via the image potential (4), the Schrödinger equation with the boundary condition $u^{im}(0) = 0$ leads to the hydrogen-like series of image states.[2] Exact solution for the ground state is

$$u_0^{im}(z) = 2\alpha_0^{3/2} z e^{-\alpha_0 z} \ , \qquad (20)$$

$$E_0^{im} = -\beta^2 \frac{e^2}{32a_0} \ , \qquad (21)$$

where

$$\alpha_0 = \beta/4a_0 \ . \qquad (22)$$

Now we include the Coulomb repulsion between electrons in the lattice and (in the $\sigma = 0$ limit) calculate its influence on the electron wave function and energy.

We shall assume that the ground-state wave function still has the same analytic dependence

$$u(z) = 2\alpha^{3/2} z e^{-\alpha z}, \quad z > 0 \qquad (23)$$

as in the noninteracting case, but the parameter α has to be determined by minimizing the functional:

$$E(\alpha) = \frac{e^2}{2}a_0\alpha^2 - \beta\frac{e^2}{4}\alpha + E_{pot}(\alpha, \sigma = 0) \ . \qquad (24)$$

The lattice potential energy $E_{pot}(\alpha,\sigma)$ is derived in the Appendix. The $\sigma=0$ limit is obtained, e.g., by substituting the operator $e^{s(\nabla_0)}$ with unity.

In Fig. 1 we show optimized values of α for various lattice parameters r_0. At low densities in the argon case α reaches the asymptotic value (α_0) already above $r_0 \sim 300$ Å, but for helium it happens at much larger distances, because the electrostatic attraction is very weak.

B. Lateral spread of the lattice electrons

Here we shall study the electrons confined at lattice sites in the potential wells of finite size and strength, and therefore with some lateral spread, but now neglecting their perpendicular size $(\alpha \to \infty)$.

In the harmonic approximation (14), which is expected to be correct at low temperatures,[15] the ground-state electron wave function takes the form

$$v_0(\rho) = \frac{1}{\sqrt{\pi}\sigma} e^{(-1/2)(\rho/\sigma)^2} , \qquad (25)$$

where the lateral spread σ of the wave function is related to the harmonic frequency ω:

$$\sigma = (\hbar/m\omega)^{1/2} . \qquad (26)$$

As an approximation we shall take a characteristic value $\omega \approx \omega_0$ close to the Brillouin zone boundary, as was defined by Bonsall and Maradudin:[14]

$$\hbar\omega_0 = \frac{e^2 2\sqrt{2}}{a_0(r_0/a_0)^{3/2}} . \qquad (27)$$

From (26) the corresponding parameter σ_0 becomes
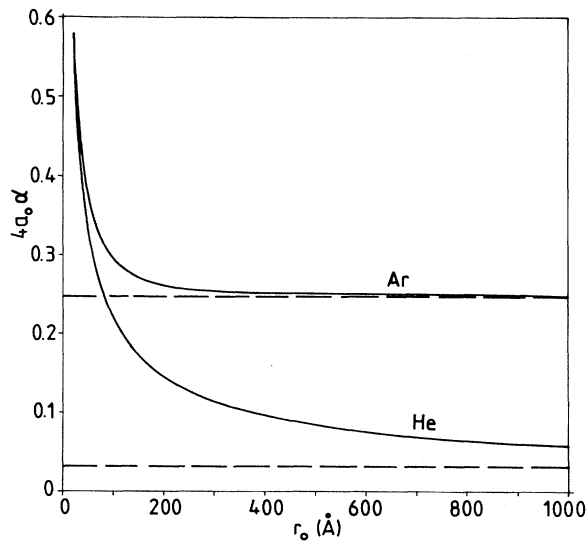
$$\left[\frac{\sigma_0}{a_0}\right] = \left[\frac{1}{2}\frac{r_0}{a_0}\right]^{3/4} \quad \text{or} \quad \left[\frac{\sigma_0}{r_0}\right] = \left[\frac{1}{8}\frac{a_0}{r_0}\right]^{1/4} . \qquad (28)$$

From Eqs. (25) and (28) we can conclude that the wave function overlap is negligible for $\sigma_0 \leq 0.2r_0$, i.e., for $r_0 \geq 40$ Å, which is practically always the case. In this way we have verified our starting (Hartree) approximation.

With the harmonic wave function (25) we have to minimize the functional

$$E(\sigma) = \frac{e^2}{2}a_0\frac{1}{\sigma^2} + E_{pot}(\alpha \to \infty, \sigma) \qquad (29)$$

in order to obtain the parameter σ. The lattice potential energy $E(\alpha,\sigma)$, derived in the Appendix, is much easier to calculate in the $\alpha \to \infty$ limit, because the function $f(x)$ now becomes a simple constant $(1-\beta)$, Eq. (A9).

Figure 2 shows the r_0 dependence of the optimized electron wave function spread σ. We also show $\sigma_0(r_0)$ given by Eq. (28), based on a simple harmonic approximation. It turns out that σ depends weakly on the properties of the substrate, so σ_0 becomes an excellent approximation for both He and Ar substrates.

The condition $r_0 > 5\sigma$ is fulfilled already for $r_0 \geq 40$ Å, which again confirms the validity of our model even in the region of high electron densities.

IV. RESULTS AND DISCUSSION

In order to find both the perpendicular and the lateral spread of the electron wave function we have to minimize the functional

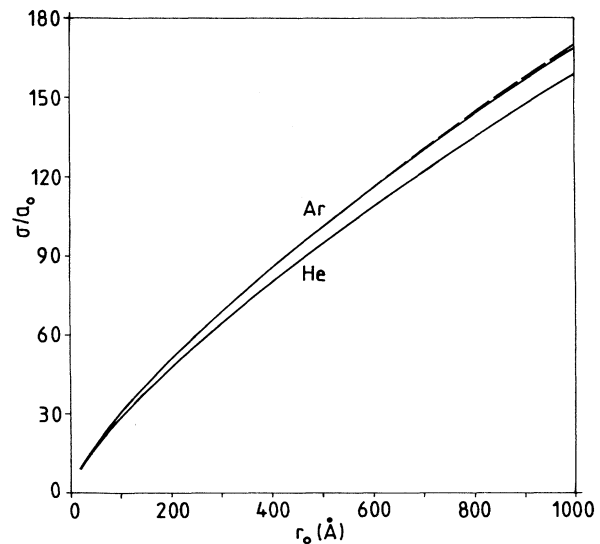$$E(\alpha,\sigma) = \langle K \rangle + \langle W^{im} \rangle + E_{pot}(\alpha,\sigma) , \qquad (30)$$

FIG. 1. Optimized values of α (in units $4a_0$) with $\sigma=0$, for helium and argon, as functions of lattice parameter r_0. The dashed lines represent the α_0 values, obtained when neglecting the electron-electron interaction: $4\alpha_0 a_0 = \beta$ takes the value 0.027 for He and 0.248 for Ar.

FIG. 2. Optimized values of σ (in units $1/a_0$) with $\alpha=\infty$, for helium and argon, as functions of lattice parameter r_0. The dashed line represents the approximative σ_0 values, which almost correspond with σ values for argon.

varying simultaneously both parameters α and σ.

The results for $\alpha(r_0)$ and $\sigma(r_0)$ are practically identical (to within 1%) to those obtained with $\sigma \to 0$ (Fig. 1) and $\alpha \to \infty$ (Fig. 2) approximations, respectively, for $r_0 > 40$ Å. The fact that the optimum values of α and σ practically do not depend on each other proves *a posteriori* the assumed factorization of the wave function (12), as pointed out in Sec. III.

In Fig. 3 we compare σ/r_0 and $\Delta z/r_0$, the ratios of the lateral and perpendicular spread parameters and r_0. Both curves have the same functional dependence: With increasing r_0 both σ and Δz increase, but their relative sizes decrease, so that for $r_0 > 10^3$ Å the electrons behave as point particles at an average distance $\langle z \rangle = 3/2\alpha$ above the dielectric surface.

It is even more significant that the lattice *compresses* at higher densities; i.e., the effective potentials confining electrons at lattice sites become more repulsive, though still harmonic. In this way the overlap of electron wave functions stays negligible even at rather higher densities, which justifies our use of the Hartree approximation in the treatment of the electrons in a Wigner lattice.

Notice that Δz is much greater than the substrate lattice constant. Therefore we believe that the microscopic effects (e.g., dispersion and decay of screening charge fluctuations, substrate lattice structure, etc.) do not play an important role in describing the electron lattice–dielectric substrate interaction.

Various energy terms and the total energy of a Wigner lattice are shown in Figs. 4(a) and 4(b). For helium, Fig. 4(a), the image term is obviously very weak and the total energy is dominated by the electron-electron interaction. For argon, Fig. 4(b), the situation is qualitatively different: The lattice potential reaches its asymptotic value rather quickly, and for $r_0 > 450$ Å it is already smaller than the image potential for this particular density.
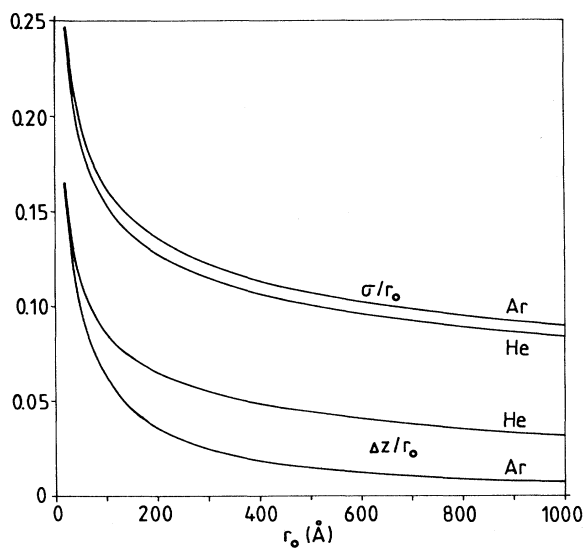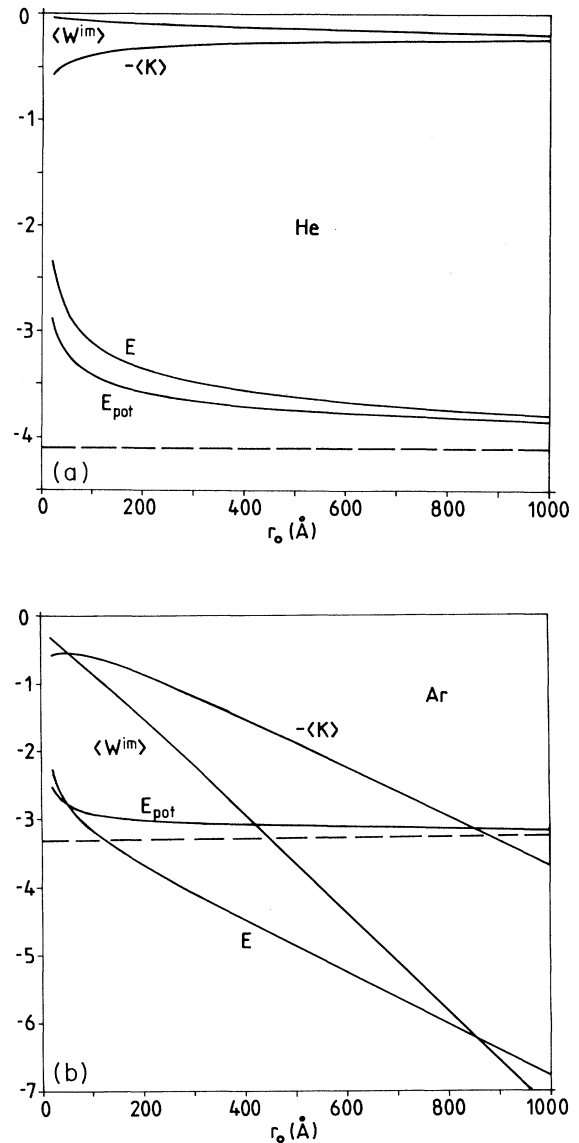

FIG. 4. Various contributions to the optimized total electron energy $E(\alpha,\sigma)$ for (a) helium and (b) argon, as functions of the lattice parameter r_0 and in units of $E_0 = e^2/r_0$. The kinetic energy term is shown with opposite sign. The dashed line represents the point-electron approximation of the electron lattice energy E_{pot} $(\alpha = \infty, \sigma = 0)$.

It turns out that the lattice potential energies are close to those calculated with $\sigma = 0$. However, kinetic energy depends both on α and σ, so the total energy thus calculated is appreciably different from the point-electron approximation E_{pot} $(\alpha \to \infty, \sigma \to 0)$ even when the image contribution is small (e.g., for helium). This means that the influence of finite σ on the total energy becomes negligible only after $r_0 > 10^3$ Å, i.e., in the region where the W^{im} term (except for small $\beta < 0.1$) dominates over the lattice potential energy. However, as the point-electron model does not (and cannot) include this W^{im} term, the validity of this model becomes doubtful for the

FIG. 3. Optimized values of Δz and σ, divided by r_0, as functions of lattice parameter r_0, for helium and argon.

whole range of densities.

Of course, the situation might be saved by an *ad hoc* shift of the electrons away from the dielectric surface. However, this shift is the consequence of exactly those finite-size effects we are addressing in this paper.

In conclusion, in this paper we have reported calculations of the ground-state energies and wave functions of electrons in a two-dimensional Wigner lattice on a dielectric substrate in the Hartree approximation. We include the effects of final electron density spread parallel and

perpendicular to the surface. Such a treatment can serve as a simple model for further investigations of two-dimensional Wigner lattices.[16]

APPENDIX: LATTICE SUM FOR THE EFFECTIVE ELECTRON-ELECTRON INTERACTION

From (11) and (12) the effective interaction among two electrons at their *regular* lateral sites (ρ_0, ρ_l) can be written in the Fourier space as

$$\langle W_{0l}^{e\text{-}e} \rangle = \frac{A}{(2\pi)^2} \int d\mathbf{k} \int dz \int dz' |u(z)|^2 |u(z')|^2 W(\mathbf{k};z,z') \int d\rho \int d\rho' e^{i\mathbf{k}\cdot(\rho-\rho')} |v(\rho-\rho_0)|^2 |v(\rho'-\rho_l)|^2 . \tag{A1}$$

the integration over (ρ, ρ') gives

$$\int d\rho \int d\rho' e^{i\mathbf{k}\cdot(\rho-\rho')} |v(\rho-\rho_0)|^2 |v(\rho'-\rho_l)|^2 = e^{i\mathbf{k}\cdot(\rho_0-\rho_l)} |v_\sigma(k)|^2 , \tag{A2}$$

where

$$v_\sigma(k) \equiv \int d\rho \, e^{i\mathbf{k}\cdot\rho} |v(\rho)|^2 = e^{(-1/4)(\sigma k)^2} .$$

Expanding

$$|v_\sigma(k)|^2 = 1 - \tfrac{1}{2}(\sigma k)^2 + \cdots \tag{A3}$$

we obtain the multipole expansion of the potential $\langle W_{0l}^{e\text{-}e} \rangle$ in terms of even powers of $\sigma/|\rho_0-\rho_l|$. Particularly, in the $\alpha \to \infty$ limit we find

$$\langle W_{0l}^{e\text{-}e} \rangle \xrightarrow[\alpha \to \infty]{} (1-\beta)\frac{e^2}{|\rho_0-\rho_l|}\left[1 + \frac{1}{2}\frac{\sigma^2}{|\rho_0-\rho_l|^2} + \cdots \right] . \tag{A4}$$

For $|\rho_0-\rho_l| \geq 5\sigma$ this expression converges very fast and σ does not influence $\langle W^{e\text{-}e} \rangle$ appreciably.

In order to obtain simple $1/\rho$ behavior appropriate for the Ewald transformation, we must take the σ dependence in front of the integral (A1). This can be done with the following identity:

$$\int d\mathbf{k}\, e^{-(1/2)(\sigma k)^2} e^{i\mathbf{k}\cdot(\rho_0-\rho_l)} = e^{s(\nabla_0)} \int d\mathbf{k}\, e^{i\mathbf{k}\cdot(\rho_0-\rho_l)} ,$$

where

$$s(\nabla_0) = \tfrac{1}{2}(\sigma\nabla_0)^2, \quad \nabla_0 \equiv \frac{\partial}{\partial x_0}\mathbf{e}_1 + \frac{\partial}{\partial y_0}\mathbf{e}_2 . \tag{A5}$$

Now we make the transformation from the Fourier space to the x space:

$$\frac{A}{(2\pi)^2} \int d\mathbf{k}\, e^{i\mathbf{k}\cdot(\rho_0-\rho_l)} \int dz \int dz' |u(z)|^2 |u(z')|^2 W(\mathbf{k};z,z') = e^2 \frac{2}{\sqrt{\pi}} \int_0^\infty dx\, e^{-(\rho_0-\rho_l)^2 x^2} f(x) . \tag{A6}$$

Obviously, in (A6) we transform the effective electron-electron interaction in the $\sigma=0$ limit. The function $f(x)$ is given by

$$f(x) = \int dz \int dz' |u(z)|^2 |u(z')|^2 (e^{-(z-z')^2 x^2} - \beta e^{-(z+z')^2 x^2}) . \tag{A7}$$

Inserting (13a) for $u(z)$ in $f(x)$, after coordinate transformation we find

$$f(x) = \tfrac{1}{8} \int_0^\infty dy\, [(y^2+3y+3) - \beta\tfrac{1}{15}y^5]e^{-y}e^{-(x/2\alpha)^2 y^2} . \tag{A8}$$

In the classical limit $f(x)$ becomes a constant:

$$\lim_{\alpha \to \infty} f(x) = 1 - \beta . \tag{A9}$$

Finally we can put $\langle W_{0l}^{e\text{-}e} \rangle$ in a convenient form:

$$\langle W_{0l}^{e\text{-}e} \rangle = e^2 \frac{2}{\sqrt{\pi}} e^{s(\nabla_0)} \int_0^\infty dx\, e^{-(\rho_0-\rho_l)^2 x^2} f(x) . \tag{A10}$$

Total electrostatic energy of an electron at $\rho_0=0$ can be written as

$$\langle W^{e\text{-}e} \rangle = \lim_{\rho_0 \to 0}\left[\sum_l \langle W_{0l}^{e\text{-}e} \rangle - \langle W_{00}^{e\text{-}e} \rangle\right] . \tag{A11}$$

Now we can use the Ewald transformation to transform the direct lattice sum over ρ_l into a sum over reciprocal lattice vectors $\mathbf{G}$:

$$\sum_l e^{-(\rho_0-\rho_l)^2 x^2} = \frac{1}{S}\frac{\pi}{x^2}\sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\rho_0} e^{-G^2/4x^2} \ . \tag{A12}$$

In a standard way we divide the potential energy in two parts: the long-range $(x < \eta)$ contribution $\langle W_G^{e\text{-}e}\rangle$ where the summation will be performed in $\mathbf{G}$ space, and the short-range $(x > \eta)$ contribution $\langle W_R^{e\text{-}e}\rangle$:

$$\langle W^{e\text{-}e}\rangle = \langle W_R^{e\text{-}e}\rangle + \langle W_G^{e\text{-}e}\rangle \ , \tag{A13}$$

$$\langle W_R^{e\text{-}e}\rangle = e^2\frac{\eta}{\sqrt{\pi}}\sum_{l\neq 0}\{e^{s(\nabla_0)}\phi_{-1/2}^R[\eta^2(\rho_0-\rho_l)^2]\}_{\rho_0=0} \ , \tag{A13a}$$

$$\begin{aligned}\langle W_G^{e\text{-}e}\rangle = {} & \langle W_{G=0}^{e\text{-}e}\rangle \\ & + \frac{e^2}{S}\frac{\sqrt{\pi}}{\eta}\sum_{\mathbf{G}\neq 0} e^{-(1/2)(\sigma G)^2}\phi_{-1/2}^G(G^2/4\eta^2) \\ & - e^2\frac{2}{\sqrt{\pi}}\int_0^\eta (e^{s(\nabla_0)}e^{-\rho_0^2 x^2})_{\rho_0=0}f(x) \ . \end{aligned} \tag{A13b}$$

$$(e^{s(\nabla_0)}e^{-(\rho_0-\rho_l)^2 x^2})_{\rho_0=0} = 1 - 2(\sigma x)^2 + 2(\sigma x)^2(\rho_l x)^2 + 4(\sigma x)^4 \ \cdots \ , $$

which leads to

$$\{e^{s(\nabla_0)}\phi_{-1/2}^R[\eta^2(\rho_0-\rho_l)^2]\}_{\rho_0=0} = \phi_{-1/2}^R(\eta^2\rho_l^2) - 2(\sigma\eta)^2\phi_{+1/2}^R(\eta^2\rho_l^2) + 2(\sigma\eta)^2[(\rho_l\eta)^2 + 2(\sigma\eta)^2]\phi_{3/2}^R(\eta^2\rho_l^2) + \cdots \ , \tag{A16}$$

$$\int_0^\eta dx (e^{s(\nabla_0)}e^{-\rho_0^2 x^2})_{\rho_0=0}f(x) = \int_0^\eta dx [1 - 2(\sigma x)^2 + 4(\sigma x)^4 + \cdots]f(x) \ . $$

The convergence is achieved for $(\sigma\eta)^2 \ll 1$.

From (19) and (A15) we find for the hexagonal lattice

$$(\sigma\eta)^2 = \left[\frac{2\pi}{\sqrt{3}}\right]\left[\frac{\sigma}{r_0}\right]^2 \ , \tag{A17}$$

so that the condition $r_0 \geq 5\sigma$ again gives very fast convergence $(\sigma\eta \leq 0.4)$.

The divergent character of the repulsive potential energy (A13) is evident in the uniform $G = 0$ term:

$$\langle W_{G=0}^{e\text{-}e}\rangle = \frac{e^2}{S}2\sqrt{\pi}\int_0^\eta dx\frac{f(x)}{x^2} \ . \tag{A18}$$

Namely, for $x\to 0$, $f(x)\sim 1-\beta$, so that the integral in (A18) diverges at the lower boundary.

This divergency has to be removed by subtracting the $k = 0$ component of the total potential energy. $\langle W^{e\text{-}e}(k=0)\rangle$ was already given in (18), but it is here convenient to rewrite it in terms of $f(x)$ as

$$\langle W^{e\text{-}e}(k=0)\rangle = \sum_l \frac{1}{A}\int d\rho\, W(\rho) = \frac{1}{S}e^2 2\sqrt{\pi}\int dx\frac{f(x)}{x^2} \tag{A19}$$

We have introduced the functions

$$\phi_n^R(z) = \int_1^\infty dt\, t^n e^{-zt}f(\eta\sqrt{t}\,) \ , \tag{A14a}$$

$$\phi_n^G(z) = \int_1^\infty dt\, t^n e^{-zt}f(\eta/\sqrt{t}\,) \ , \tag{A14b}$$

which both reduce to the standard Misra functions if f is a constant (as in the $\alpha\to\infty$ limit).

Obviously $\langle W^{e\text{-}e}\rangle$ should not depend on the choice of the parameter η and we choose it to be

$$\eta = (g_0/2r_0)^{1/2} \ , \tag{A15}$$

so that direct and lattice sums converge equally fast. In this way it is enough to take only the first two terms in the sums (A13a) and (A13b).

The operator $e^{s(\nabla_0)}$ gives simply the factor $e^{-(1/2)(\sigma G)^2}$ when operating on $\mathbf{G}$ terms. To evaluate the expressions in curly brackets in (A13) we use the expression

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in order to show explicitly that $\langle W^{e\text{-}e}(k=0)\rangle$ cancels the divergency in the $G=0$ term of $\langle W_G^{e\text{-}e}\rangle$:

$$\langle W_{G=0}^{e\text{-}e}\rangle - \langle W^{e\text{-}e}(k=0)\rangle = -\frac{e^2}{S}2\sqrt{\pi}\int_\eta^\infty dx\frac{f(x)}{x^2} \ . \tag{A20}$$

In this way the lattice potential energy

$$E_{\text{pot}}(\alpha,\sigma) \equiv \langle W^{e\text{-}e}\rangle - \langle W^{e\text{-}e}(k=0)\rangle \tag{A21}$$

becomes finite and attractive, which stabilizes the electron lattice.

Let us notice that for localized electrons we find

$$E_{\text{pot}}(\alpha\to\infty,\sigma\to 0) = -(1-\beta)4.2134e^2/r_0 \ . \tag{A22}$$

This point-electron result was already obtained, for $\beta=0$, by Bonsall and Maradudin.[14]

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