Influence of the envelope function on the ground-state energy of quasi-two-dimensional Wigner solids

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(Received 11 May 1992)

At sufficiently low density, quasi-two-dimensional electron systems in their ground state form Wigner solids. In previous studies of the ground-state energy of such systems (in the absence of an applied magnetic field), the finite extension of electron wave functions in the direction perpendicular to the interface plane has not been considered. The effect of the finite width of envelope functions on the ground-state energy of quasi-two-dimensional Wigner solids is studied in this paper. We evaluate the total Coulomb energy using numerically efficient Jacobi θ-function methods, for a variety of assumed crystal structures. The ground-state energy is found to be rather sensitive to the envelope wave-function width but the crystal structure remains hexagonal.

I. INTRODUCTION

Strongly correlated interacting many-electron systems of reduced dimensionality have become increasingly important in recent years. Progress in fabrication techniques have resulted in the development of new low-dimensional electron systems and devices. In quasi-two-dimensional systems, the intriguing quantum features of these materials have been the subject of extensive experimental studies in the low-temperature regime. Theoretical interest has been correspondingly intense.

Our present interest is focused on the quasi-two-dimensional electron systems which exist at a GaAs–$Al_xGa_{1-x}As$ heterojunction or the interface regions in a Si metal-oxide-semiconductor field-effect transistor.[1,2] We are specifically concerned with the ground-state energy at very low density and in zero applied magnetic field. Strictly two-dimensional electron systems have been studied previously within the context of the usual electron gas model.[3–6] At sufficiently low density, the electrons condense and the ground state is a crystalline Wigner solid. In terms of the parameter r_s given by the area per particle $A/N = \pi(r_s a_B)^2 = 1/n$, where a_B is the effective Bohr radius, the energy per particle in the Wigner solid is

$$\varepsilon = E/N = \frac{c_1}{r_s} + \frac{c_{3/2}}{r_s^{3/2}} + \frac{c_2}{r_s^2} + \cdots . \tag{1}$$

The first term is the static Coulomb energy of the Wigner solid and the leading correction term is due to the zero-point energy of the phonons. At sufficiently low density (large r_s), the ground-state energy is dominated by the static Coulomb energy. The numerical values of the Madelung constant, c_1, and the other coefficients depend on the precise crystal lattice structure of the Wigner solid. It has not been found possible to predict the correct lattice structure of the Wigner solid by general arguments. This is a common situation and not restricted to purely electronic systems. Instead, specific structures are assumed and the energy is calculated for each of these structures. Of the various crystal structures studied for the two-dimensional Wigner solid, the hexagonal lattice has the lowest Coulomb energy and is also stable with respect to lattice vibrations.[5] It is believed that the ground state of a *strictly* two-dimensional electron system is a Wigner solid with hexagonal lattice structure in the low density limit.

Of course, the electron systems which exist at interfaces in systems of present interest are not strictly two dimensional (planar) but have a finite extent in the z direction perpendicular to the plane of the interface. The precise electron density distribution $n(x,y,z)$ may still be taken, ideally, to be uniform in the x,y plane but the extension of the electron distribution in the z direction is determined by details of the confinement mechanism. In principle, the resulting electron density distribution can be obtained by an appropriate self-consistent procedure. The effective Schrödinger equations for the z dependence of the electron wave functions are

$$\left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} + V_{\text{eff}}(z)\right]\zeta_n(z) = \varepsilon_n\zeta_n(z), \tag{2}$$

where $V_{\text{eff}}(z)$ is the total potential energy (including any fixed, induced, image charge, and other contributions) which is to be determined in the course of self-consistently solving Eq. (2) for the density distribution and m^* is an effective mass for motion in the z direction. In practice, a much simpler approximate procedure is invoked in cases where only the lowest surface subband energy state is occupied. An approximate $n = 0$ subband wave function is taken to be of the form

$$\zeta_0(z) = (2b^3)^{-1/2} z e^{-z/2b}, \tag{3}$$

and the parameter b, which gives the length scale of the electron distribution, is determined variationally by minimizing the total energy.[7]

After some simplification, the minimizing value of b is

found to be

$$b = \left(\frac{2\epsilon\hbar^2}{33\pi m^* e^2 n}\right)^{1/3}, \tag{4}$$

where ϵ is the background dielectric constant. In terms of the effective Bohr radius $a_B = \hbar^2/[m^*(e^2/\epsilon)]$, the width is

$$b = \left(\frac{2a_B}{33\pi n}\right)^{1/3} = \left(\frac{2r_s^2}{33}\right)^{1/3} a_B, \tag{5}$$

where r_s was given above by the total number of electrons per unit area of the interface.[8] In the present application, the most relevant parameter is the ratio of the width of the envelope function to the average spacing of electrons in the plane

$$\beta = b/(r_s a_B) = \left(\frac{2}{33 r_s}\right)^{1/3} \tag{6}$$

which is largely independent of material properties such as the effective mass and dielectric constant.

Equation (6) is a convenient universal form describing the influence of finite width of the envelope function in the very-low-density regime of the Wigner solid. Note that the effect of multiple valleys or isospin degeneracy[9] can become significant whenever details of the kinetic energy need to be taken into account. One such case is Si(100) at electron densities near the critical density for Wigner crystallization.[10] Using standard data for $Al_xGa_{1-x}As$ and Si(100), reasonable values of β are found to be in the range $0.1 \lesssim \beta \lesssim 0.5$.

The presence of an additional length scale b in addition to $r_s a_B$ has significant effect on the energetics of the quasi-two-dimensional system. Denoting coordinates in the plane by $\mathbf{r} = (x, y)$, we can consider the effective interparticle interaction to be

$$v_{\rm eff}(\mathbf{r}-\mathbf{r}') = \int_0^\infty dz \int_0^\infty dz' \zeta_0^2(z)\zeta_0^2(z') \times [(\mathbf{r}-\mathbf{r}')^2 + (z-z')^2]^{-1/2}. \tag{7}$$

Clearly, $v_{\rm eff}(\mathbf{r}-\mathbf{r}')$ is substantially reduced in strength, particularly at small separations, relative to the strictly two-dimensional $e^2/|\mathbf{r}-\mathbf{r}'|$. In addition, for two fixed lattice points in the plane, the mean square interparticle separation is increased from r_{ij}^2 to

$$\int_0^\infty dz \int_0^\infty dz' \zeta_0^2(z)\zeta_0^2(z')[r_{ij}^2 + (z-z')^2] = r_{ij}^2 + 6b^2. \tag{8}$$

Now the ground-state crystal structure of a given system is known to be very sensitive to details of the interparticle interaction. In the *strictly* two-dimensional case, the ground state of the Wigner solid has a close-packed-hexagonal (also often referred to as triangular) crystal structure, as discussed above. As a result of the softening of the effective interactions and the increase in the mean square interparticle separations described above, it is not clear, *a priori*, whether the ground-state crystal structure of the quasi-two-dimensional Wigner solid is also hexagonal when the envelope function is taken into account. A definitive answer requires an explicit calculation. In addition, irrespective of the crystal structure, it is of interest to determine how sensitive the ground-state energy is to the width of the envelope function.[11] This information will be useful in subsequent applications.

The objective of this work has been to provide answers to these two questions. In Sec. II, the Coulomb energies are determined numerically for a variety of simple crystal structures of the quasi-two-dimensional Wigner solid. The sensitivity of these energies to the width of the envelope function is shown. The final section contains a discussion of the results.

II. LATTICE SUMS FOR GROUND-STATE ENERGY

To be specific, our calculation will be phrased in terms of a simple picture of a heterojunction. The electron layer is confined near the plane $z = 0$ and extends into the region of $z > 0$ due to the finite width of the envelope function. Overall charge neutrality is provided by the donor ions which are modeled by a homogeneous layer of positive charge of area density ρ_d, situated at $z = -b_d$. In order to isolate the long-range contributions (which will all ultimately cancel for the neutral interface system in the $q \to 0$ limit), we write the total Coulomb energy as

$$E_c = \lim_{q\to 0}[E_{dd}(q) + E_{ee}(q) + 2E_{ed}(q)], \tag{9}$$

where

$$E_{dd}(q) = \frac{1}{2}\int d^2r \int d^2r' \rho_d^2 \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} = \frac{e^2 A \rho_d^2 \pi}{q} = \frac{Ne^2}{q(r_s a_B)^2}, \tag{10}$$

$$E_{ee}(q) = \frac{1}{2}\int d^2r \int d^2r' \rho_e(\mathbf{r})\rho_e(\mathbf{r}') e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \int_0^\infty dz \int_0^\infty dz' \zeta_0^2(z)\zeta_0^2(z') \frac{e^2}{[(\mathbf{r}-\mathbf{r}')^2 + (z-z')^2]^{1/2}}, \tag{11}$$

and

$$E_{ed}(q) = -\frac{1}{2}\int d^2r \int d^2r' \rho_d \rho_e(\mathbf{r}') e^{iq\cdot(\mathbf{r}-\mathbf{r}')} \int_0^\infty dz' \zeta_0^2(z') \frac{e^2}{[(\mathbf{r}-\mathbf{r}')^2 + (b_d+z')^2]^{1/2}}$$
$$= -\frac{\sqrt{\pi} e^2 A \rho_d^2}{2} \int_0^\infty dy\, y^{-3/2} e^{-q^2/4y} \int_0^\infty dz' \zeta_0^2(z') e^{-y(z'+b_d)^2}$$
$$= -\frac{\pi e^2 \rho_d^2 A}{2q} e^{-qb_d} \frac{2!}{(qb+1)^3}$$
$$= -\frac{e^2 N}{(r_s a_B)^2}\left(\frac{1}{q} - 3b - b_d + O(q)\right). \tag{12}$$

$E_{dd}(q)$ is the energy of the donor ions, $E_{ee}(q)$ is the energy of the electron layer, and $E_{ed}(q)$ is the energy due to coupling of the ions and electrons. Although the charge distribution of the donor ions is uniform, the electrons are in a crystalline state. Integrating over the z degree of freedom is elementary but the integration over the electron distribution in the plane requires summation over the lattice points of the Wigner solid.

The lattice sum technique based on the Jacobi θ functions and their imaginary transforms is ideal to calculate ground-state energies of different lattice structures of heterojunctions or electron inversion layers.[12,13] As in Eq. (11), we first write the Coulomb potential energy via an integral transform

$$V_{ee}(\mathbf{r}-\mathbf{r}') = [|\mathbf{r}-\mathbf{r}'|^2 + |z-z'|^2]^{-1/2} = \int_0^\infty \frac{dy}{\Gamma(1/2)} y^{-1/2} e^{-y|\mathbf{r}-\mathbf{r}'|^2 - y|z-z'|^2}. \tag{13}$$

By decomposing the lattice into rectangular sublattices indicated with sublattice vectors $\boldsymbol{\rho}_i$, position vectors of electrons are given as

$$\mathbf{r} = ma_1\hat{x} + na_2\hat{y}, \quad \mathbf{r}' = (m'a_1 + \rho_i^x)\hat{x} + (n'a_2 + \rho_i^y)\hat{y},$$

where m, m', n and n' are integers, and a_1 and a_2 are lattice constants of sublattices.

$$\int d^2r \int d^2r' V_{ee}(\mathbf{r}-\mathbf{r}') e^{iq\cdot(\mathbf{r}-\mathbf{r}')} = \int_0^\infty \frac{dy}{\sqrt{\pi}} y^{-1/2} e^{-y|z-z'|^2}$$
$$\times N \sum_{l=m-m'}{}' \sum_{k=n-n'}{}' \exp[-y(\rho_i^x + la_1)^2 + iq_x(\rho_i^x + la_1)]$$
$$\times \exp[-y(\rho_i^y + ka_2)^2 + iq_y(\rho_i^y + ka_2)]. \tag{14}$$

The Jacobi θ function is defined as

$$\theta(z, X) = \sum_{l=-\infty}^{\infty} e^{2\pi l z} e^{-\pi l^2 X}. \tag{15}$$

Advantages of introducing $\theta(z; X)$ functions are that the θ function converges well for large X, and we are also able to obtain convenient well-convergent formulas for the small-X region by applying the Jacobi imaginary transformation from which the Coulomb singular part at $q \to 0$ can be rigorously extracted.[12,13] Thus, the Coulomb energy of electrons obtained using Eq. (14) in Eq. (11) can be separated into a large y part and a small y part given by

$$E_{ee}(q) = E_{ee}^{>}(q) + E_{ee}^{<}(q), \tag{16}$$

where

$$N^{-1}E_{ee}^{>}(q) = \frac{1}{2}\sum_i \frac{e^2}{\sqrt{\pi}} \int_{y_0}^\infty dy\, y^{-1/2} f(y,b) \left[e^{-y\rho_i^2 + iq\cdot\rho_i} \prod_{\alpha=x,y} \theta\left(-\frac{(2\rho_i^\alpha y - iq_\alpha)a_\alpha}{2\pi}; \frac{a_\alpha^2 y}{\pi}\right) - \delta_{i,0}\right] \tag{17}$$

and

$$N^{-1}E_{ee}^{<}(q) = \frac{1}{2}\sum_i \left(\frac{\sqrt{\pi} e^2}{a_1 a_2} \int_0^{y_0} dy\, y^{-3/2} f(y,b) e^{-q^2/4y} \left\{ \left[\prod_{\alpha=x,y} \theta\left(+i\frac{(2\rho_i^\alpha y - iq_\alpha)}{2a_\alpha y}; \frac{\pi}{a_\alpha^2 y}\right) - 1\right] + 1\right\} \right.$$
$$\left. -\delta_{i,0}\frac{e^2}{\sqrt{\pi}} \int_0^{y_0} dy\, y^{-1/2} f(y,b) e^{-y\rho_i^2 + iq\cdot\rho_i} \right) \tag{18}$$

with

$$f(y,b)=\int_0^\infty dz\int_0^\infty dz'\zeta_0^2(z)\zeta_0^2(z')e^{-y|z-z'|^2}$$
$$=\frac{1}{4b^6}\left\{-\frac{b^2}{8y^2}+\frac{3b^4}{4y}+\left(-\frac{b^3}{2y}+\frac{b}{8y^2}+\frac{3b^5}{2}\right)\frac{e^{1/4yb^2}}{2\sqrt{y}}\Gamma\left(\frac{1}{2},\frac{1}{4yb^2}\right)\right\}. \tag{19}$$

At the limit $q\to 0$, $E_{ee}^{<}(q)$ becomes

$$N^{-1}E_{ee}^{<}(q)=\frac{1}{2}\sum_i\left\{\frac{\sqrt{\pi}e^2}{a_1a_2}\int_0^{y_0}dy\,y^{-3/2}f(y,b)\left[\prod_{\alpha=x,y}\theta\left(+i\frac{2\rho_i^\alpha y}{2a_\alpha y};\frac{\pi}{a_\alpha^2 y}\right)-1\right]-\frac{\sqrt{\pi}e^2}{a_1a_2}\int_{y_0}^\infty dy\,y^{-3/2}f(y,b)\right\}$$
$$-\frac{e^2}{2\sqrt{\pi}}\int_0^{y_0}dy\,y^{-1/2}f(y,b)+N^{-1}E_{ee}^{\rm hom}(q), \tag{20}$$

where $E_{ee}^{\rm hom}(q)$ is the Coulomb energy corresponding to a homogeneous electron distribution,

$$N^{-1}E_{ee}^{\rm hom}(q)=\frac{\sqrt{\pi}e^2n_l}{2a_1a_2}\int_0^\infty dy\,y^{-3/2}f(y,b)e^{-q^2/4y}$$
$$=\frac{e^2}{4(r_sa_B)^2q}\left(\frac{3/2}{qb+1}+\frac{3/2}{(qb+1)^2}+\frac{1}{(qb+1)^3}\right)$$
$$=\frac{e^2}{(r_sa_B)^2}\left(\frac{1}{q}-\frac{15b}{8}+\cdots\right). \tag{21}$$

Here, $a_1a_2/n_l=\pi(r_sa_B)^2$ and n_l is the number of sublattices. Note that the Coulomb singularity $(1/q)$ in Eq. (21) cancels exactly with the corresponding $1/q$ terms of $E_{dd}(q)$ and $E_{ed}(q)$ [Eqs. (10) and (12), respectively].

The results of our numerical calculations of the structure-dependent contributions to $E_{ee}(q\to 0)$ for particular two-dimensional lattice structures are summarized in Table I(a). The *total* interface energy per electron

TABLE I. (a) The results of numerical calculations of the lattice-structure-dependent contributions to $N^{-1}E_{ee}(q=0)$ are given for different values of parameter $\beta=b/r_sa_B$ for hexagonal (hex), square (sq), centered rectangular (CR) with the various ratios of lattice constants (a_2/a_1), rectangular (rec) with different lattice constant ratios, and honeycomb (HC) lattice structures. The energies are measured in effective Hartree units, e^2/r_sa_B. (b) The *total* interface energies per electron for hexagonal (hex), square (sq), centered rectangular (CR) with the various ratios of lattice constants (a_2/a_1), rectangular (rec) with different lattice constant ratios, and honeycomb (HC) lattice structures are given for the various values of parameter β. The energies are measured in effective Hartree units, e^2/r_sa_B.

β	0	10^{-3}	10^{-2}	10^{-1}	1
			(a)		
hex	−1.106103	−1.104230	−1.087592	−0.941894	−0.416275
sq	−1.100244	−1.098372	−1.081738	−0.936369	−0.414441
CR($\sqrt{2}$)	−1.104080	−1.102208	−1.085571	−0.939987	−0.415642
CR(0.95)	−1.100352	−1.098480	−1.081846	−0.936471	−0.414475
rec($\sqrt{3}$)	−1.042844	−1.040971	−1.024376	−0.882335	−0.396359
rec($\sqrt{2}$)	−1.078201	−1.076329	−1.059709	−0.915604	−0.407513
rec(0.95)	−1.099774	−1.097901	−1.081267	−0.935925	−0.414294
HC	−1.068417	−1.066541	−1.049925	−0.906213	−0.403941
			(b)		
hex	−1.106103	−1.100105	−1.046432	−0.529394	3.708725
sq	−1.100244	−1.094247	−1.040488	−0.523869	3.710559
CR($\sqrt{2}$)	−1.104080	−1.098083	−1.044321	−0.527487	3.709358
CR(0.95)	−1.100352	−1.094355	−1.040596	−0.523971	3.710525
rec($\sqrt{3}$)	−1.042844	−1.036846	−0.983126	−0.469835	3.728641
rec($\sqrt{2}$)	−1.078201	−1.072204	−1.018459	−0.503104	3.717487
rec(0.95)	−1.099774	−1.093776	−1.040017	−0.523425	3.710706
HC	−1.068417	−1.062416	−1.008675	−0.493713	3.721059

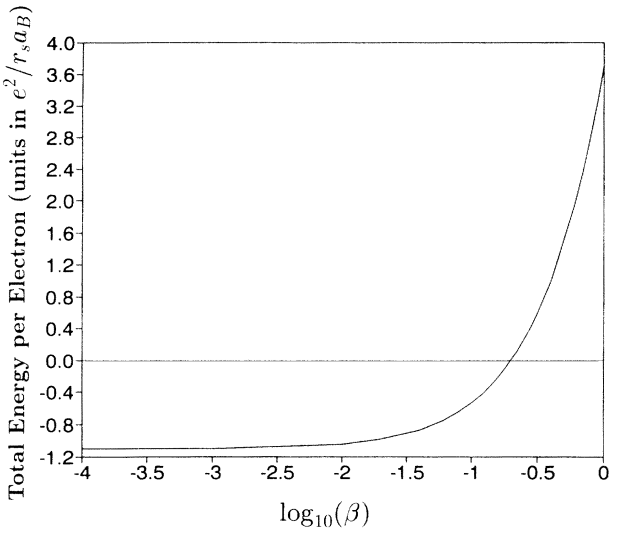

FIG. 1. The total interface energy per electron in a hexagonal lattice structure is shown as a function of the parameter $\beta = b/r_sa_B$, in logarithmic scale.

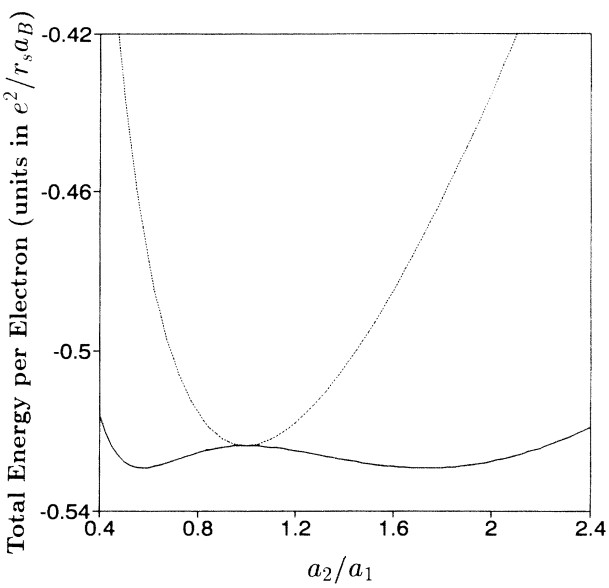

FIG. 2. Lattice structure dependence of the total interface energy per electron at $\beta = 0.1$ is shown. The solid curve is the energy of the centered rectangular lattice as a function of the ratio (a_2/a_1) of lattice constants, and the dashed curve is the energy of the rectangular lattice as a function of the lattice constant ratio. Two minima of the solid curve correspond to the hexagonal lattice structure at the ratio $\sqrt{3}$ or $1/\sqrt{3}$. The minimun in the dashed curve corresponds to the square lattice structure.

is obtained according to Eqs. (12) and (21), by adding

$$(2b_d + 33b/8)e^2/(r_sa_B)^2 \tag{22}$$

to the entries of Table I(a). The contribution $2b_de^2/(r_sa_B)^2$ is strictly constant and will be ignored in the following. The contribution $(33b/8)e^2/(r_sa_B)^2 = (33/8)\beta e^2/r_sa_B$ is added to the structure-dependent contributions of Table I(a) to yield the total interface energy per electron listed in Table I(b). It is seen that the total energy increases as β increases for all cases studied but that the hexagonal lattice structure continues to exhibit the lowest energy. In fact, there is no crossing of any of the total energy curves for any of the lattice structures (in the physical range of β values) although the total energies of different lattice structures become closer to each other as β increases. In Fig. 1, we plot the total energy per electron for the hexagonal lattice structure as a function of the envelope-function width parameter. The dependence of the total energy of the centered rectangular lattice on the ratio of lattice constants a_2/a_1 is shown in Fig. 2. The two equivalent minima at $a_2/a_1 = \sqrt{3}$ and $1/\sqrt{3}$ correspond to the hexagonal structure while the local maximum at $a_2/a_1 = 1$ corresponds to the square lattice structure. The corresponding total energy curve for the rectangular lattice is also shown.

To test the sensitivity of these results to the precise form of $\zeta_0(z)$, we replaced the standard Fang-Howard envelope function by a Gaussian

$$\zeta_G(z) = \frac{e^{-z^2/2b_G^2}}{(\sqrt{\pi}b_G)^{1/2}} \tag{23}$$

and repeated all of the numerical calculations. Then Eq. (12) becomes

$$E_{ed}(q) = -\frac{e^2A\rho_d^2}{2}\int_0^\infty dy\, y^{-3/2}e^{-q^2/4y}\int_{-\infty}^\infty \frac{dz}{b_G}e^{-(z/b_G)^2}e^{-y|z+b_d|^2}$$
$$= -\frac{e^2N}{(r_sa_B)^2}\left\{\frac{1}{q} - \frac{b_G}{\sqrt{\pi}}e^{-(b_d/b_G)^2} - b_d\Phi\left[\left(\frac{b_d}{b_G}\right)^2\right] + O(q)\right\}, \tag{24}$$

where Φ is the probability function. Equation (19) becomes

$$f(y, b_G) = (2b_G^2y + 1)^{-1/2} \tag{25}$$

and Eq. (21) is then replaced by

$$N^{-1}E_{ee}^{\rm hom}(q) = n_l\frac{\sqrt{\pi}e^2}{2a_1a_2}\int_0^\infty dy\, y^{-3/2}\frac{e^{-q^2/4y}}{\sqrt{2b_G^2y+1}}$$
$$= \frac{e^2}{(r_sa_B)^2}\left(\frac{1}{q} - \sqrt{\frac{2}{\pi}}b_G + O(q)\right). \tag{26}$$

TABLE II. (a) The results of numerical calculations of the lattice-structure-dependent contributions to $N^{-1}E_{ee}(q=0)$ are given for different values of Gaussian parameter $\beta_G = b_G/r_s a_B$ for hexagonal (hex), square (sq), centered rectangular (CR) with the various ratios of lattice constants (a_2/a_1), rectangular (rec) with different lattice constant ratios, and honeycomb (HC) lattice structures. The energies are measured in effective Hartree units, $e^2/r_s a_B$. (b) The *total* interface energies per electron for hexagonal (hex), square (sq), centered rectangular (CR) with the various ratios of lattice constants (a_2/a_1), rectangular (rec) with different lattice constant ratios, and honeycomb (HC) lattice structures are given for the various values of Gaussian parameter β_G. The energies are measured in effective Hartree units, $e^2/r_s a_B$.

β_G	0	10^{-3}	10^{-2}	10^{-1}	1
			(a)		
hex	−1.106103	−1.105305	−1.098164	−1.030292	−0.623733
sq	−1.100244	−1.099447	−1.092306	−1.024496	−0.620352
CR($\sqrt{2}$)	−1.104080	−1.103283	−1.096142	−1.028291	−0.622566
CR(0.95)	−1.100352	−1.099555	−1.092414	−1.024603	−0.620414
rec($\sqrt{3}$)	−1.042844	−1.042046	−1.034912	−0.967731	−0.587219
rec($\sqrt{2}$)	−1.078201	−1.077404	−1.070266	−1.002693	−0.607627
rec(0.95)	−1.099774	−1.098976	−1.091836	−1.024030	−0.620080
HC	−1.068417	−1.067616	−1.060478	−0.992976	−0.601314
			(b)		
hex	−1.106103	−1.104975	−1.094859	−0.997242	−0.293239
sq	−1.100244	−1.099116	−1.089001	−0.991446	−0.289857
CR($\sqrt{2}$)	−1.104080	−1.102953	−1.092837	−0.995242	−0.292071
CR(0.95)	−1.100352	−1.099225	−1.089109	−0.991553	−0.289919
rec($\sqrt{3}$)	−1.042844	−1.041716	−1.031607	−0.934681	−0.256724
rec($\sqrt{2}$)	−1.078201	−1.077073	−1.066961	−0.969643	−0.277133
rec(0.95)	−1.099774	−1.098646	−1.088531	−0.990981	−0.289585
HC	−1.068417	−1.067286	−1.057173	−0.959927	−0.270819

Numerical results for the electron energy and the total interface energy (with b_d set equal to zero) for this Gaussian "envelope function" are given in Table II. The effect of the parameter b_G is somewhat weaker than the effect of b in the envelope function, but it is obvious that the hexagonal structure is again most stable. Our previous conclusions regarding the stability of the hexagonal structure are thus not overly sensitive to details of the envelope function.

III. CONCLUSION

The width of the envelope function has a very significant effect on the ground-state energy of the quasi-two-dimensional Wigner solid in the very-low-density regime. We have evaluated the total Coulomb energy using numerically efficient Jacobi θ-function methods for a variety of assumed crystal structures. Numerical results are given for a range of values of the ratio of the envelope-function width to the planar interparticle spacing $\beta = b/r_s a_B$. We find that the total energy curves for different crystal structures never cross as a function of β. Thus, so long as the electron density is low enough that the Coulomb energy is dominant, and the structure is also stable with respect to lattice vibrations, the ground-state crystal structure of the quasi-two-dimensional Wigner solid is hexagonal just as it is for the *strictly* two-dimensional Wigner solid. We find the same conclusions when the standard Fang-Howard envelope function is replaced by a Gaussian. We expect these results to be general, for physical values of β, so long as the planar and perpendicular degrees of freedom are not coupled. On the other hand, although the crystal structure itself is not modified, the numerical value of the ground-state energy is very sensitive to the envelope-function width. Typically, the Coulomb energies increase sharply and even change sign as β increases from $\beta = 0$ (strictly two dimensional) to $\beta = 0.5$. This sensitivity indicates that it will be essential to take the width of the envelope function into account when considering details of the phase diagram of the low-density electron system.

ACKNOWLEDGMENTS

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada and by the Hamilton Foundation (N.M.F.). We also acknowledge informative discussions with A. H. MacDonald and M. Rasolt.

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