Angular pinning and domain structure of a two-dimensional Wigner crystal in a III-V semiconductor

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We consider acoustic-phonon-mediated electron-electron interaction in III-V semiconductors. It is shown that this is strongly anisotropic and influences the properties of the two-dimensional Wigner crystal. The resulting domain structure of the Wigner solid and the surface tension between the domains are semiquantitatively investigated.

Many interesting phenomena determined by electronic correlations in the two-dimensional (2D) electron systems such as the fractional quantum Hall effect or the possibility of formation of a 2D Wigner crystal are widely investigated experimentally and theoretically.¹ It has been shown (e.g., Refs. 2-7) that Wigner crystallization can occur in a magnetic field for sufficiently small filling of the Landau level. However, the phase diagram of the 2D correlated electronic system is not yet well known. One important difficulty of the theory of 2D electronic phases is that the Coulomb interaction is long range, and the thermodynamical properties of the system only weakly depend on its local structure. Therefore, the different electronic phases have almost the same value of the energy. For example, in the 2D Wigner crystal⁸ the difference in the energies per particle of the hexagonal (minimum) and the square (maximum) lattices is only $0.0104(e^2/\epsilon)\sqrt{n_c}$ (that is 1/200 of their values), where e is the elementary charge, n is the concentration of the carriers, and ϵ is the dielectric constant. In this situation a weak external perturbation can strongly influence the system. We suppose that this perturbation in III-V semiconductors can be attributed to the electron-phonon coupling. These T_d -symmetry crystals are piezoelectrics. Hence, acoustic phonons cause a long-range electric field giving rise to a phonon-mediated electron-electron interaction. Theoretical investigations of the electron-phonon interaction in piezoelectrics were performed extensively.⁹⁻¹² It has been shown in Ref. 10 that the electron-acousticphonon coupling is analogous to the electron-photon interaction in quantum electrodynamics with the appropriate "charge" determined by the crystal properties. Most of the studies¹⁰⁻¹² assumed an isotropic electron-phonon coupling vertex. Below we investigate the interaction of the electrons via the acoustic phonons using the full expression for this anisotropic coupling. The strength of the resulting anisotropic interaction is determined by two different charges, in order of magnitude coinciding with the one introduced in Ref. 10. (An analogous problem was considered for isotropic optical phonons in Ref. 13.) In the two-dimensional case the anisotropy is determined by the crystallographic plane of the 2D system. We analyze the effect of this interaction on the properties of the 2D Wigner crystal, generalizing the approach of Ref.

14. We demonstrate that this interaction considerably affects the 2D Wigner solid, although it is much weaker than direct Coulomb repulsion. We always use $\hbar = 1$.

In the III-V crystal the piezoelectric tensor is reduced to one constant κ_{14} ,¹⁵ and the Hamiltonian of the electron-acoustic phonons coupling is written as

$$\begin{split} \hat{H}_{e-p} &= \sqrt{\frac{2\pi}{V}} \frac{\kappa_{14}}{\sqrt{\rho}} \frac{e}{\epsilon} \sum_{\vec{k},\vec{q},\mu} \frac{1}{\sqrt{qs_{\mu}}} [e_x e_y d^z + e_z e_x d^y \\ &+ e_y e_z d^x] \left(\hat{a}_{\vec{q},\mu} + \hat{a}^+_{-\vec{q},\mu} \right) \hat{b}^+_{\vec{k}+\vec{q}} \hat{b}_{\vec{k}}. \end{split}$$
(1)

Here the index $\mu = l, t$ corresponds to the phonon branch (longitudinal and transverse one), s_{μ} is the μ -branch speed of sound, ρ is the crystal density, V is its volume, \vec{k}, \vec{q} are the electron and phonon momentum, respectively, $\vec{d} = \vec{q}/q$, and \vec{e} is the polarization of the phonon. $\hat{a}^+_{-\vec{q},\mu}$ and $\hat{b}^+_{\vec{k}+\vec{q}}$ are the phonon and electron creation operators, respectively.

The procedure of calculating the pair interaction between the charges is well known.¹⁶ Because the Hamiltonian in Eq. (1) is \vec{e} and \vec{q} dependent, we have to average over the directions of the intermediate phonon momenta and polarizations. After averaging over \vec{e} directions for the longitudinal, and \vec{d} and \vec{e} directions for the transverse phonons, we integrate with respect to q in order to obtain the interaction potential. In the static limit, for which the electrons are at rest (the applicability of this approximation will be discussed below), the additional potential is written as the sum of the invariants of the T_d -symmetry group:

$$\varphi_p\left(\vec{R}\right) = -\frac{1}{R} \left[e_0^2 I_0 + e_4^2 I_4 + e_6^2 I_6 \right], \qquad (2)$$

where $\vec{R} = \vec{n}R$ is the radius vector between the particles. The invariants I_j and the charges e_j are

$$I_0 = 1, \quad I_4 = n_x^2 n_y^2 + n_z^2 n_y^2 + n_x^2 n_z^2, \quad I_6 = n_x^2 n_y^2 n_z^2, \quad (2a)$$

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$$e_{\mu}^{2} = \frac{\kappa_{14}^{2}}{\rho s_{\mu}^{2}} \frac{e^{2}}{\epsilon^{2}}, \quad e_{0}^{2} = \frac{e_{t}^{2}}{4},$$

$$e_{4}^{2} = \frac{3}{16} \left(3e_{l}^{2} - e_{t}^{2} \right), \quad e_{6}^{2} = \frac{45}{16} \left(e_{t}^{2} - e_{l}^{2} \right),$$
(2b)

respectively. Since $s_l > s_t$, the "transverse" charge e_t is larger than the "longitudinal" one, e_l . Because they are of the same order of magnitude, for the estimations we can use e_l .

The investigation of the 2D electron system, which is located on a crystallographic plane characterized by the normal vector $\vec{\nu}$, requires a projection of the function $\varphi_p(\vec{R})$ on this plane. We treat two types of $\vec{\nu}$ for which these projections can be written in a simple form.

(A) Plane with the normal vector $\vec{\nu} = (0, \nu_1, \nu_2), \nu = 1$. In this case an in-plane vector \vec{n} is written as

$$ec{n} = ec{e_1}\cos\psi + ec{e_2}\sin\psi,$$

$$\vec{e_1} = (1,0,0), \ \vec{e_2} = (0,-\nu_2,\nu_1).$$
 (3)

The projections of the invariants on this plane are

$$I_4(\vec{n}|\vec{\nu}) = \frac{1}{8} \left(1 + 3\nu_1^2 \nu_2^2 \right) + \frac{1}{2} \nu_1^2 \nu_2^2 \cos 2\psi \\ - \frac{1}{8} \left(1 - \nu_1^2 \nu_2^2 \right) \cos 4\psi$$
(3a)

 and

$$I_6(\vec{n}|\vec{\nu}) = \frac{1}{16}\nu_1^2\nu_2^2\left(1 + \frac{1}{2}\cos 2\psi - \cos 4\psi - \frac{1}{2}\cos 6\psi\right).$$
(3b)

(B) For $\vec{\nu} = (\nu_1, \nu_1, \nu_2)$ the basic vectors in the plane are given by

$$\vec{e}_1 = \frac{1}{\sqrt{2}} \left(-\nu_2, -\nu_2, 2\nu_1 \right), \quad \vec{e}_2 = \frac{1}{\sqrt{2}} \left(-1, 1, 0 \right).$$
 (4)

Hence we obtain

$$\begin{split} I_4\left(\vec{n}|\vec{\nu}\right) &= \frac{1}{4} \left[1 - \frac{1}{8} \left(3\nu_2^2 - 1 \right)^2 \right] \\ &+ \frac{1}{8} \left(3\nu_2^2 - 1 \right) \left[\left(1 - \nu_2^2 \right) \cos 2\psi \right. \\ &\left. - \frac{1}{4} \left(\nu_2^2 - 3 \right) \cos 4\psi \right], \end{split} \tag{4a}$$

 and

$$\begin{split} I_{6}\left(\vec{n}|\vec{\nu}\right) &= \frac{1}{16}\nu_{1}^{2}\left(\frac{5}{2}\nu_{2}^{4} - \nu_{2}^{2} + \frac{1}{2}\right) + \frac{1}{64}\nu_{1}^{2}\left(3\nu_{2}^{2} - 1\right) \\ &\times \left[\left(5\nu_{2}^{2} + 1\right)\cos 2\psi + 2\left(\nu_{2}^{2} + 1\right)\cos 4\psi\right] \\ &+ \frac{1}{64}\nu_{1}^{2}\left(\nu_{2}^{2} + 1\right)^{2}\cos 6\psi. \end{split} \tag{4b}$$

We can see that the projections are strongly anisotropic and reflect the symmetry of the plane. As a result of the anisotropy, the properties of the crystal determined by this interaction are sensitive to its *local order* because at large distances the role of the ψ -dependent terms is negligible. Therefore, it can affect the transition of the correlated electron system to the Wigner solid or the charge density wave states.

We now discuss the applicability of the static limit calculations. A sufficient condition for the validity of this approximation is $ms_l \gg \sqrt{n_c}$, where m is the effective mass of the carrier. For the electron systems where $m \sim 0.1m_0$ (m_0 is the free electron mass) and $s_l \sim 5 \times 10^5$ cm/sec, this condition is fulfilled for concentrations $n_c < 10^{10}$ cm⁻² (these systems have been investigated in Ref. 17). Another situation occurs in the hole systems. Here the effective mass of the carrier is determined by the width of the 2D structure¹⁸ as a result of the coupling between subbands of heavy and light holes. The mass can be rather large ($m \sim m_0$), yielding $n_c \sim 10^{11}$ cm⁻².

Now let us consider how this interaction affects the properties of the Wigner solid located on the highsymmetry planes. The basic vectors of the Wigner lattice are given by $\vec{b}_1 = (a_1, 0)$ and $\vec{b}_2 = (a_1/2, a_2/2)$. The invariants I_0 and $I_4(\vec{n}|\vec{\nu})$ on the [111] plane of hexagonal symmetry only lead to a weak isotropic renormalization of the charge, which for our purpose can be neglected. From the I_6 invariant [Eq. (4b)] we get the anisotropic potential

$$\varphi_a(\vec{r}) = -\frac{e_h^2}{r}\cos 6\psi, \qquad e_h^2 = \frac{e_6^2}{108},$$
 (5)

where \vec{r} is the in-plane radius vector and ψ is the angle between \vec{r} and the projection of the (001) vector on the [111] plane. Numerical calculations give the energy per particle for the hexagonal (E_h) and the square (E_s) lattices due to this interaction: $E_h \approx -2.24 e_6^2 \sqrt{n_c}$ and $E_s = 0$, respectively. Because of the inequality $E_h < E_s$, the Wigner crystal is stabilized. Consider the square symmetry [001] plane, where $I_6(\vec{n}|\vec{\nu}) = 0$. Then $\varphi_a(\vec{r})$ can be written as

$$\varphi_a(\vec{r}) = \frac{e_s^2}{r}\cos 4\psi, \qquad e_s^2 = \frac{e_4^2}{8},$$
 (6)

where ψ is the angle between \vec{n} and the x direction. We have a competition of two interactions: the strong direct Coulomb repulsion tends to form the hexagonal lattice, while the relatively weak anisotropic interaction favors the square one. The corresponding piezoelectric energy of the square and hexagonal lattices are $E_s \approx -1.04e_4^2 \sqrt{n_c}$ and $E_h = 0$, respectively. The lattice with the minimum total (Coulomb + piezoelectric) energy is a centered rectangular one with $1/\sqrt{3} < a_2/a_1 < 1$.

The pair interactions in Eqs. (5) and (6) depend on the ψ angles. Hence, the total energy of the Wigner solid should be dependent on its orientation with respect to the III-V lattice. This effect is macroscopic, since it is determined by the number of particles in the Wigner crystal. Therefore, the system should be sensitive to this weak coupling. From this statement we can draw two conclusions.

(1) The Wigner crystal loses the rotational symmetry, and hence, should be pinned with respect to rotations in the plane. A simple estimation based on Eqs. (2b) and (6) shows that if $n_c \sim 10^{10} \text{ cm}^{-2}$ and $e_l \sim 10^{-3} e$ then the domains with the number of the particles N > $10^3(T/K)$ should be pinned, while the smaller ones are still randomly oriented. Pinning of the Wigner crystal by impurities as a result of breaking of the translational invariance is widely investigated (e.g., Refs. 6 and 19). The breaking of rotational invariance means that a new branch should be observed in the spectrum of collective excitations of the 2D Wigner crystal. The corresponding frequency of the small angular vibrations of the Wigner solid Ω is evaluated as $e_l n_c^{3/4} / \sqrt{m}$. Supposing $e_l / e \sim 10^{-3}$, $m \sim 0.1 m_0$, and $n_c \sim 10^{11}$ cm⁻² we obtain values of Ω in the order 1–10 GHz. This frequency is close to the predicted for the Wigner glasses.¹⁹

(2) Because the Wigner crystal on the [001] plane has four minimal energy positions [where the angle θ between the \vec{b}_1 and the (100) axis is $\pi l/2$, l = 0, 1, 2, 3], it is possible to obtain a domain structure with different orientations of the basic vectors. We qualitatively evaluate the width and the surface tension of the domain wall. For this purpose we write the energy of the wall per unit length as

$$\Phi \sim \int \left\{ \alpha \left[d heta(x')/dx'
ight]^2 + eta [\cos 4 heta(x') - 1]
ight\} dx',$$
 (7)

where the axis x' is perpendicular to the wall. The first term in the brackets of Eq. (7) is the elastic energy of the deformed crystal determined by the Coulomb forces, while the second one depends on the Wigner solid orientation with respect to its host lattice. The constants α and β can be expressed in the terms of the system parameters as follows:

$$\alpha \sim \frac{e^2}{\epsilon a_c}, \qquad \beta \sim \frac{e_4^2}{a_c^3},$$
(7a)

where $a_c \sim 1/\sqrt{n_c}$ is the Wigner lattice constant. We should minimize Φ with respect to the function $\theta(x')$ taking into account the boundary conditions $\theta(\infty) = 0, \theta(-\infty) = \pi/2$. A variational procedure leads to the sine-Gordon equation. For a qualitative estimation we obtain the wall width

$$w \sim \sqrt{\frac{\alpha}{\beta}} \sim a_c \frac{e}{\sqrt{\epsilon}e_4} \gg a_c,$$
 (7b)

and the surface tension

$$\sigma \sim \sqrt{\alpha\beta} \sim \frac{ee_4}{\sqrt{\epsilon}} n_c. \tag{7c}$$

We can see that σ is small enough, while w is rather large. Estimation according to Eq. (7c) at $n_c \sim 10^{10} \text{ cm}^{-2}$ gives $\sigma \sim 10^{-2} K/10^{-5} \text{cm}$. The small tension means that the Wigner crystal can have a developed domain structure. This structure is specific only for the [001] plane because in the other cases the domain structure is impossible [this follows from the analysis of Eqs. (3) and (4)].

Summarizing the most relevant aspects of the paper, we formulate the following statements. First, the exchange by the acoustic phonons in III-V semiconductors leads to an anisotropic interaction between the charges. Second, this interaction manifests itself via the properties of the 2D electronic systems, especially in the Wigner solid region. For instance, the stable lattice on the [001] plane is between the hexagonal and square ones. For the strong enough interaction the square one is preferable. On the [111] plane this interaction stabilizes the hexagonal Wigner crystal. However, this effect is small because $e_l/e \sim 10^{-3}$. Third, as result of the anisotropy of the electron-electron interaction the basic vectors of the Wigner crystal should be oriented on the plane by a specific way to minimize the total energy of the system. This effect is macroscopic and can be experimentally investigated. For example, the electron diffraction recently used by Harris et al.²⁰ for investigation of a 2D Wigner solid should be sensitive to the domains orientation and can be used for this purpose. On the [001] plane this interaction can lead to a domain structure with small surface tension and wide walls. Therefore, this system can have an orientational disorder, in some aspects analogous to "orientational glasses."²¹

Note, that the qualitative statements and estimations discussed above are based mainly on symmetry arguments. Therefore, they are model independent and not strongly sensitive to the detailed properties of the Wigner solid.

The theory of 2D melting²² shows that the symmetry of the substrate influences the melting process. In Ref. 22 this effect is determined by the fluctuations induced by the substrate symmetry. In our case substrate symmetry leads to the new interaction within the melted crystal. Comparison of these cases is interesting and will be presented elsewhere.

Note, that in our consideration the weak phononmediated interaction occurs on the background of the strong Coulomb one. Further investigation of these systems, for instance, by methods like Monte Carlo simulation can shed additional light on the properties of the strongly correlated 2D systems.

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