Two-Dimensional Wigner Crystal in Anisotropic Semiconductor

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We investigate the effect of mass anisotropy on the Wigner crystallization transition in a two-dimensional (2D) electron gas. The static and dynamical properties of a 2D Wigner crystal have been calculated for arbitrary 2D Bravais lattices in the presence of anisotropic mass, as may be obtainable in Si MOSFETs with (110) surface. By studying the stability of all possible lattices, we find significant change in the crystal structure and melting density of the electron lattice with the lowest ground state energy.

One of the most unexpected discoveries in the 2D electron systems in semiconductor structures is the possibility of a metal-insulator transition (MIT) first suggested by experiments of Kravchenko et al. in high mobility Si metal-oxide-semiconductor field-effect transistors (MOSFETs) in zero magnetic field [1]. Later, a number of groups have reported possible MITs in 2D electron or hole systems in several different semiconductor heterostructures, as well as in MOSFETs [2]. However, a genuine MIT in two dimensions is in contradiction to the scaling theory of localization, which predicts that in the absence of electron-electron (or hole-hole) interactions no true metallic behavior is possible in two dimensions with pure potential scattering [3]. In fact, no fundamental principle requires that such a scaling argument holds in the presence of strong interactions, which can be measured by the ratio of the Coulomb energy to Fermi energy, expressed by the dimensionless parameter $r_s = m^* e^2/\hbar^2 \sqrt{\pi n}$, and there have been a number of suggestions that this is the case [10–12]. Theoretical models not involving MIT have also been proposed [13–15]. Of all the experimental systems, the critical $r_s$ varies from 5 in Si$_{0.88}$Ge$_{0.12}$ [2] up to 35 in GaAs/AlGaAs [8], which clearly suggests that the Coulomb interactions are certainly not negligible, but in fact may be the dominating scale.

It is well known that 2D electrons crystallize into a triangular lattice (Wigner crystallization) in the low density limit where electron-electron interactions dominate. In an ideally clean 2D system, the critical $r_s$ is predicted by Tanatar and Ceperley to be 37 [9]. This is in good agreement with the range of the critical $r_s$ observed in the recent experiments.

In this paper, we have carried out a further test on the relevance of the Wigner crystallization phenomenon to the putative 2D MITs by exploring the effect of mass anisotropy on Wigner crystallization, since mass anisotropy can be presented in Si- or Ge-based semiconductor devices. In particular, we have studied the ground state energy of arbitrary 2D Bravais lattice with anisotropic mass. To the best of our knowledge, no result on such properties of 2D Wigner crystal with anisotropic mass has been published so far.

The ground state energy of a lattice in the low density limit, where exchange process are negligible, can be written as the sum of static Coulomb energy and vibrational zero-point energy. With the aid of Ewald’s transformation [16], we can write the static ground state energy per electron of a Bravais lattice as a sum over its lattice sites $r_0$:

$$E_s = -\frac{1}{N} \sum_{i<j} e^2 \left| r_0^i - r_0^j \right|$$

$$= -\frac{2e^2}{\sqrt{\pi}} \left[ 2 - \sum_{r^0 \neq 0} \phi_{-1/2} \left( \frac{\pi}{v} |r^0|^2 \right) \right],$$

where $\phi_n(x)$ is the Misra function [2].

and $v$ is the area of the primitive unit cell of the direct lattice. We assume the existence of a neutralizing background of positive charges to avoid the divergence in the evaluation of the static energy, which is independent of the mass anisotropy. In a harmonic approximation, the spectrum of lattice vibrations is determined by

$$\mathcal{H} = \sum_i \sum_{\alpha} \frac{p_\alpha(r^0_i)^2}{2m_\alpha} + \frac{1}{2} \sum_{i,j} \sum_{\alpha,\beta} u_{\alpha}(r^0_i) \Phi_{\alpha\beta}(r^0_i, r^0_j) u_{\beta}(r^0_j),$$

where $u(r^0) = r - r^0$ is the deviation from equilibrium of the electron whose equilibrium site is $r^0$. The atomic force constants $\Phi_{\alpha\beta}(r^0_i, r^0_j)$ are defined by

$$\Phi_{\alpha\beta}(r^0_i, r^0_j) = \begin{cases} -\frac{\partial^2 v(r)}{\partial r_\alpha \partial r_\beta} & |r_i - r_j| = r^0_i - r^0_j, \ i \neq j \\ \sum_{k \neq i} \frac{\partial^2 v(r)}{\partial r_\alpha \partial r_k} & |r_i - r_k| = r^0_i - r^0_k, \ i = j \end{cases}$$

with $v(r) = e^2/r$. The normal mode frequencies $\omega_\lambda(\mathbf{q})$ are solutions of the 2D eigenvalue problem:

$$M \omega_\lambda^2(\mathbf{q}) \epsilon_\lambda = D(\mathbf{q}) \epsilon_\lambda,$$
where the dynamical matrix \( \mathbf{D}(\mathbf{q}) \) is given by
\[
\mathbf{D}(\mathbf{q}) = \sum_{\mathbf{R}^0} \Phi(\mathbf{R}^0)e^{-i\mathbf{q}\cdot\mathbf{R}^0}.
\]  
(6)

In anisotropic systems, \( \mathbf{M} \) is a \( 2 \times 2 \) matrix. The dynamical ground state energy can be obtained by integrating zero-point energies of all modes within the Brillouin zone.

Bonsall and Maradudin did a comprehensive study on the ground state energies of five different crystal structures, including triangular lattice and square lattice, for isotropic 2D electrons [18]. They found that the triangular lattice has the lowest energy in low density limit, 
\[
E_0 = -\frac{2.21}{r_s} + \frac{1.63}{r_s^{3/2}},
\]  
(7)
in units of \( \text{Ryd} = m^*e^4/h^2 \). In Eq. (7), the first term comes from the Coulomb interactions between electrons sitting on the lattice sites, while the second term is from the harmonic oscillations of electrons around their equilibrium positions. They also pointed out that the transverse branch of the dispersion relation is pure imaginary for certain directions in the square lattice, implying a dynamical instability of this lattice.

FIG. 1. 2D Bravais lattices can be mapped to points within the shaded area. Dynamically stable lattices are mapped to only one tenth of the irreducible area.

In the presence of the mass anisotropy, the ground state may not necessarily be one of the most symmetric lattices. Therefore, we have developed a systematic method to explore the ground state energies of 2D Bravais lattices with different electron concentrations and mass anisotropy. First, we map an arbitrary Bravais lattice to a point on a 2D plane by the following scheme. From an arbitrary lattice site, which is chosen to be origin, one can choose an arbitrary pair of two non-collinear lattice vectors that span the Bravais lattice. If one rotates and scales the lattice so that one of the two primitive vectors lies along x-axis normalized to unit length, the end point of the other lattice vector represents the 2D lattice structure. However, a lattice can be mapped to infinite number of points due to arbitrary choice of primitive vectors. One can reduce the area of points by choosing two shortest vectors from the origin with the second shortest one placed along x-axis. Thus, different lattices are represented by points in the upper positive quadrant as shown in Fig. 1. Using reflection symmetry, however, all the points can be confined by the y-axis and the two circles shown (the shaded area) in Fig. 1. The three corners (0,1), \( \left( \frac{1}{2}, \frac{\sqrt{3}}{2} \right) \) and (0,0) represent square lattice, triangular lattice, and quasi-one-dimensional lattice, respectively. We can then sample 2D lattices by applying a rectangular mesh on the area and calculating the ground state energy on each grid point, which can be uniquely mapped back to a 2D Bravais lattice.

Applying Bonsall and Maradudin’s calculations on all sampled lattices with isotropic mass, we found that most lattices have imaginary vibrational modes, therefore are unstable. Under our mapping, only lattices around the triangular lattice are stable, which occupies roughly 10% of the reduced zone, as shown in Fig. 1. Using symmetry, one can actually show the triangular lattice is the center of all stable lattices. Within the stable area the triangular lattice has the lowest energy for \( r_s > 25 \), which is slightly below the Wigner crystallization density \( r_s = 37 \pm 5 \) predicted in quantum Monte Carlo calculations [14]. When \( r_s = 25 \), the lattice represented by point A (0.27, 0.95) starts to have lower energy than the triangular lattice, whose ground state energy is found to be
\[
E_{0A} = -\frac{2.206}{r_s} + \frac{1.594}{r_s^{3/2}}.
\]  
(8)

Since point A is adjacent to the unstable area, this implies that Wigner lattice is no longer the ground state of the 2D electron system.

We have studied different ratios between longitudinal mass \( m_l \) and transverse mass \( m_t \). In this paper, we present results of \( m_l/m_t = 3 \), which is approximately the mass ratio in silicon (110) surface structures [21]. We use the geometric mean of the two mass components as the effective mass in calculating \( r_s \). The relative orientation of the lattice vectors with respect to the principle axes of anisotropic mass has also been taken into consideration. Figure 2 compares the dispersion relation of the anisotropic triangular lattice with that of the isotropic lattice. Mass anisotropy lifts the 2-fold degeneracy at J-point thus the longitudinal branch as well. The ground state energy for triangular lattice for \( m_l/m_t = 3 \) therefore becomes
\[
E_{0T} = -\frac{2.212}{r_s} + \frac{1.694}{r_s^{3/2}}.
\]  
(9)

Compared with Eq. (1), one concludes the mass anisotropy leads to an increase in the total lattice vibrational energy.
FIG. 2. Dispersion curves for triangular lattice with anisotropic mass ratio $m_l/m_t = 3$. Frequency is measured in units of $(m^* e^4 / h^3 r_s^{3/2})$.

Since the electrostatic ground state energy is independent of mass anisotropy, one expects that at low enough density, the triangular lattice remains as the lowest energy configuration. However, just for $m_l/m_t = 3$ even at very low density, specially $r_s < 1000$, we find that the lattice with the lowest ground state energy starts to shift along one of the circular curve that confines the reduced lattice area towards the quasi-one-dimensional lattice. It is understandable that a lattice can stretch along the axis of the smaller mass to reduce the longitudinal energy of lattice vibration. This trend is shown in the enlarged stable area in Fig. 3.

Fig. 4 shows the plots of the ground state energy for different lattices represented by the two circular curves (A-T-B) at different $r_s$ for $m_l/m_t = 3.0$. When $r_s = 100$, the ground state energy is minimized at a point along curve TB. We expect 2D electrons crystallize in the lattice structure mapped to this point at such density. When $r_s = 80$ the lattice with the lowest energy moves to the corner of the stable area, B, which connects with the area of unstable lattices. The comparison of the phonon dispersion curves of the triangular lattice and the lattice mapped to point B suggests that, by crystallizing in less symmetric lattice, the electrons gain larger energy in longitudinal modes than the loss in transverse modes. When $r_s = 60$, the ground state energy decreases linearly when approaching point B from the stable area along the circular curve TB, which implies that no stable lattice can be formed at this density. The comparison of the ground state energies suggests that the Wigner crystallization density for ideally clean 2D anisotropic electrons, such as silicon (110) surface electrons, is much lower than that predicted for an isotropic system.

In this calculation we have neglected quantum mechanics of the electrons (i.e. electronic exchange energy). While this may have a quantitative effect, it is unlikely to completely alter our basic conclusion that $r_s$ of the Wigner crystallization transition increases with mass anisotropy. This is especially true since the $r_s$ of interest ($\sim 80$) is very large, where exchange energies are smallest.

To summarize, we have found the ground state of 2D electron system has strong dependence on the mass anisotropy. In a pure system, anisotropic electrons re-
quire larger spacing to form Wigner lattice so as to sta-
blize the long wavelength transverse modes. It would be
interesting to see if this dramatic reduction in Wigner
crystal density can be observed in extremely clean Si
(110) MOSFET, in which our calculations estimate the
critical density, in terms of $r_s$, can be as large as 80.

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