Absence of Wigner Crystallization in Graphene.

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Graphene, a single sheet of graphite, has attracted tremendous attention due to recent experiments which demonstrate that carriers in it are described by massless fermions with linear dispersion. In this note, we consider the possibility of Wigner crystallization in graphene in the absence of external magnetic field. We show that the ratio of potential and kinetic energy is independent of the carrier density, the tuning parameter that usually drives Wigner crystallization and find that for given material parameters (dielectric constant and Fermi velocity), Wigner crystallization is not possible. We comment on the how these results change in the presence of a strong external magnetic field.

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Graphene is a single sheet of carbon atoms which can be extracted from graphite by micro-mechanical cleavage. Various theoretical and experimental studies of this 2-dimensional system have shown that its properties are markedly different from those of the conventional 2-dimensional electron gas (2DEG) formed in semiconductor heterostructures. The carriers in such a 2DEG are well described by Fermi liquid theory, and have quadratic dispersion at small momenta, \( E_k = \frac{\hbar^2 k^2}{2m^*} \), where \( m^* \) is the band mass. Carriers in graphene, on the other hand, have a band structure in which electron and hole bands touch at two points in the Brillouin zone. This, combined with the hexagonal lattice structure of graphene, lead to linear dispersion at small momenta, \( E_k = \hbar v_C k \). Therefore the carriers behave as “massless” Dirac particles with characteristic velocity \( v_C \sim 10^6 \text{ m/s} \). This difference in the character of quasi-particles - massive quadratically dispersing vs. massless linearly dispersing - gives rise to a host of remarkable phenomena including unusual quantum Hall effects and \( \pi \) Berry phase.

Another interesting aspect of graphene is that it is a better realization of two dimensional system. The conventional 2DEG is formed in semiconductor quantum wells where the width of the quantum well is usually around 100 - 300 Å. Various properties of such a 2DEG have been extensively studied using primarily transport measurements. However, it has not been amenable to local probes such as a scanning tunneling microscope (STM), because the 2DEG is buried about 1000 Å from the sample surface. In graphene, on the other hand, the width of the effective quantum well is approximately 5 - 10 Å (distance between two graphene sheets in graphite), and the 2DEG is amenable to local probes including those which will allow the study of inhomogeneous states. In addition, the density and the polarity of carriers in graphene can be adjusted simply by changing the gate voltage; something that is not possible in conventional semiconductor heterojunctions.

Here, we investigate the possibility of Wigner crystallization in graphene. Following the pioneering work of E. Wigner, a Wigner crystal has become one of the extensively studied phases of conventional 2DEG at low densities. This state appears when electrons localize and form a crystal to minimize the potential energy, while paying the concommitant kinetic energy cost which arises from localization, as the density of carriers is lowered. Theoretical studies predict that Wigner crystallization in conventional 2DEG occurs at \( r_s \sim 37 \), where \( r_s = \frac{a_B}{a_B} \) is the mean interparticle spacing and \( a_B \) is the Bohr radius. In the presence of a strong magnetic field, the kinetic energy of electrons is quenched at filling factors \( \nu \leq 1 \); in other words, electrons can localize without paying the kinetic energy cost. Therefore, Wigner crystallization is facilitated by the magnetic field. The experimental study of the quantum Hall effect in conventional 2DEG has shown the existence of the Wigner crystal phase at filling factors \( \nu \leq 1/5 \), deduced from vanishing Hall and longitudinal conductivity.

The situation in case of graphene is not yet fully explored. In the absence of a magnetic field, graphene shows metallic behavior over a large range of density for both polarities. In the quantum Hall regime it shows finite Hall and longitudinal conductivity, although only integer filling factors have been explored. Hence, it is appropriate to ask if Wigner crystallization occurs in graphene. In this note we show that Wigner crystal phase is not possible in graphene except in the presence of an external magnetic field.

First, we present a heuristic argument for our result. Our discussion is limited to low temperatures \( T \to 0 \); at finite temperatures, a translationally broken symmetry state will be destroyed by fluctuations in two dimensions. We know that the Wigner crystal phase is formed...
as a result of the competition between the potential energy \( E_p \) and kinetic energy \( E_k \) of the system. When \( E_p \gg E_k \) the crystallization occurs. We estimate the two energies in graphene as follows. Assuming localization of \( E \) in conventional 2DEG, Wigner crystallization occurs for crystal. It is worthwhile to remember at this point that \( E \) suppressing the dielectric constant to increase the ratio of the two energies, and obtain numerical estimates for.

In the following, we present a microscopic calculation of localization to an insulator by reducing density of carriers. Since it is known experimentally that graphene is not an insulator, it will not undergo Wigner crystalization to an insulator by reducing density of carriers, (which, in turn, is related to the density of carriers), the potential energy is given by \( E_p \sim (e^2/\epsilon l)nA \) where \( n \) is the density of carriers, \( A \) is the area of the system, and \( \epsilon \) is the static dielectric constant of graphene. The kinetic energy, on the other hand, will be given by \( E_k \sim \hbar v_G(2\pi/l)nA \) where \( \hbar v_G = 5.8 \) eV\( \cdot A \) is the velocity of massless Dirac fermions. Hence, the ratio of these two energies is

\[
\frac{E_p}{E_k} \sim \frac{e^2}{\hbar v_G} \frac{1}{\epsilon}.
\]

Two important observations thus follow immediately: i) The ratio is independent of the density of carriers, a situation very different from that in the conventional 2DEG ii) The ratio depends on only two (tunable) material parameters, \( \epsilon \) and \( v_G \).

Thus, for graphene, we find that energetics of the system do not depend on the carrier density. In particular, since it is known experimentally that graphene is not an insulator, it will not undergo Wigner crystallization to an insulator by reducing density of carriers. In the following, we present a microscopic calculation of the two energies, and obtain numerical estimates for suppressing the dielectric constant to increase the ratio \( E_p/E_k \), which may drive the system towards a Wigner crystal. It is worthwhile to remember at this point that in conventional 2DEG, Wigner crystallization occurs for \( E_p/E_k = r_s \sim 3.7 \).

Now we will proceed with more detailed estimates of the kinetic and potential energy. In the ground state \( |F\rangle \), the kinetic energy of the system is given by

\[
E_k = \langle F|\hat{H}_0|F\rangle = \hbar v_G \sum_{k\lambda} k\langle F|a_{k\lambda}^\dagger a_{k\lambda}|F\rangle = \hbar v_G 4A k_F^3
\]

where \( \sum_{\lambda} = 4 \) is the sum over the spin and valley degeneracy, \( a_{k\lambda}^\dagger \) creates an electron with momentum \( k \) (measured from the Dirac point), and the Fermi momentum \( k_F \) is related to the carrier density by \( n = k_F^2/\pi \). Therefore, the kinetic energy becomes

\[
E_k = \frac{2\sqrt{3}}{3} \hbar v_G An^{3/2}.
\]

Similarly the potential energy is calculated as follows

\[
E_p = \frac{e^2}{2\epsilon} \sum_{kpq\lambda_1\lambda_2} \sum_{\lambda_3} \frac{2\pi}{q} \langle F|a_{k+q+\lambda_3}^\dagger a_{p-q-\lambda_2}^\dagger a_{p+\lambda_2} a_{k+\lambda_3}|F\rangle = \frac{4\sqrt{3}\pi e^2}{3\epsilon} A n^{3/2}
\]

So their ratio is given by

\[
\frac{E_p}{E_k} = \frac{4e^2}{\hbar v_G} \frac{1}{\epsilon}
\]

and is independent of density of carriers as expected. For the experimental parameters, \( \epsilon = 4.7 \) and \( \hbar v_G = 5.8 \) eV\( \cdot A \), the ratio \( E_p/E_k \simeq 0.32 \). Thus, kinetic energy is roughly three times bigger than the potential energy, and the carriers prefer to be delocalized in a uniform state. For Wigner crystallization, we need \( E_p/E_k \gg 1 \).

Next we consider the dependence of this ratio on the two tunable parameters, \( \epsilon \) and \( v_G \). To this end, we first calculate the change in the static dielectric constant, \( \epsilon(q \rightarrow 0, \omega = 0) \) due to the spin-orbit coupling \( \Delta_{so} \) in graphene [10]. The spin-orbit coupling in graphene is estimated to be as high as \( 4 \) meV [17]. Therefore, following the derivations in Ref[11], we calculate the dielectric constant for \( 0 \leq \Delta_{so} \leq 5 \) meV.

At \( \omega = 0 \), the dielectric functional \( \epsilon(q) \) can be written as

\[
\epsilon(q) = 1 + U_0(q)\Pi(q)
\]

where \( U_0(q) = 2\pi e^2/q \) is the two-dimensional Coulomb interaction in Fourier space and \( \Pi(q) \) is the static bare particle-hole propagator

\[
\Pi(q) = -4 \sum_{\lambda,\lambda',k} |g_{k}^{\lambda,\lambda'}(q)|^2 \frac{f[E_{k+q}^\lambda] - f[E_k^\lambda]}{E_{k+q}^\lambda - E_k^\lambda + i\eta}
\]

Here, the factor of 4 takes into account of the spin and valley degeneracy, the index \( \lambda = \pm 1 \) denotes the two bands, and the vertex factor is given by [11],

\[
|g_{k}^{\lambda,\lambda'}(q)|^2 = \frac{1}{2} (1 + \frac{\lambda\lambda'\sin \alpha_k + q \sin \alpha_k (k + q \cos \theta)}{|k + q|} + \lambda\lambda' \cos \alpha_k q \cos \alpha_k)
\]

where \( \theta \) is the angle between \( k \) and \( q \). \( \alpha_k \) is defined through, \( \tan \alpha_k = \frac{k_{\lambda}q_{\lambda'} + k_{\lambda'}q_{\lambda}}{\Delta_{so}} \). \( E_k^\pm = \pm \sqrt{\Delta_{so}^2 + \hbar^2 v_G^2 k^2} \) is the energy spectrum of the carriers in \( \pm \) bands and \( f[E_k^\lambda] \) is the Fermi distribution function.

At low temperatures \( T \rightarrow 0 \), only the interband scattering contributes to \( \epsilon(q) \). Figure 1 shows the dependence of \( \epsilon \) on \( \Delta_{so} \) evaluated numerically. We see that the dielectric constant decreases sharply with an increase in \( \Delta_{so} \). When the spin orbit interaction energy is zero, the dielectric constant is \( \epsilon = 4.7 \), whereas, \( \epsilon \simeq 1.1 \) for \( \Delta_{so} = 4 \) meV. The decrease in dielectric constant increases the energy ratio to \( E_p/E_k \simeq 1.4 \). Even in the extreme case, \( \epsilon = 1 \) (no screening whatsoever), the maximum value of the ratio is \( E_p/E_k \approx 1.5 \), which is smaller than the ratio \( E_p/E_k = r_s \sim 3.7 \) required for Wigner crystallization in a conventional 2DEG.
Figure 1: Static dielectric constant $\epsilon(q \to 0, \omega = 0)$ as a function of the spin-orbit interaction energy $\Delta_{so}$. We have used $\hbar v_G = 5.8$ eVÅ. We find that at $\Delta_{so} = 4$ meV, $\epsilon \simeq 1.1$ approaches the minimum value possible $\epsilon = 1$.

The second parameter $v_G$ can be tuned by putting strain on the system. In a tight-binding model, the velocity $v_G$ is related to the tunneling amplitude $t$ and the lattice constant $a$ by $v_G = 3ta/2$. By straining the sample, the lattice constant increases linearly whereas the tunneling amplitude decreases exponentially, thus effectively decreasing the velocity of massless carriers. How effective this method will be in increasing the ratio $E_p/E_k$, depends upon the elastic properties of graphene; however, it seems unlikely that the velocity $v_G$ can change by an order of magnitude that will be required for Wigner crystallization. Therefore, we conclude that Wigner crystal phase is absent in graphene. The kinetic energy is always comparable to the potential energy, and both scale as $n^{3/2}$ with the carrier density. This peculiar dependence arises because of the linear dispersion of carriers.

We note that these arguments will not be valid in the presence of a strong magnetic field. In that case, the system develops Landau levels with energies $E_m = \pm \hbar v_G/l_B\sqrt{2m}$ where $l_B$ is the magnetic length. Each Landau level is macroscopically degenerate. Therefore at small filling factors $\nu \ll 1$, we expect the carriers to undergo Wigner crystallization as there is no concomitant increase in the kinetic energy cost associated with the localization (This conclusion is robust for the $n = 0$ Landau level, where the eigenfunctions are identical to those in the lowest Landau level of a conventional 2DEG). The critical value of the filling factor $\nu_c$ at which the Wigner crystallization occurs will have to be determined by a microscopic calculation, and is the subject of future work.

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