Chiral symmetry breaking in graphene

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Abstract
The question of whether the Coulomb interaction is strong enough to break the sublattice symmetry of undoped graphene is discussed. We formulate a strong coupling expansion where the ground state of the Coulomb Hamiltonian is found exactly and the kinetic hopping Hamiltonian is treated as a perturbation. We argue that many of the properties of the resulting system would be shared by graphene with a Hubbard model interaction. In particular, the best candidate sublattice symmetry-breaking ground state is an antiferromagnetic Mott insulator. We discuss the results of some numerical simulations which indicate that the Coulomb interaction is indeed subcritical. We also point out the curious fact that if the electron did not have spin degeneracy, the tendency to break chiral symmetry would be much greater and even relatively weak Coulomb interactions would likely gap the spectrum.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Some of the original work in the prehistory of graphene [1] was motivated by an attempt to find an analogue in condensed matter physics of some very nice structures that, in the early 1980s, had emerged in the study of relativistic quantum field theories in three space–time dimensions. These included the appearance of Chern–Simons terms and topological mass for gauge fields [2, 3], the parity anomaly [4–6] and the use of the index theorem [4, 7–11] to learn about features of the spectrum of the Dirac Hamiltonian. When graphene was discovered and made readily available in the laboratory [12], as luck would have it, many of its features turn out to be well described by free (2 + 1)-dimensional relativistic fermions with an emergent $U(4)$ symmetry. The index theorem plays a role. It determines the degeneracy of the states at zero energy, when the electrons are exposed to an external magnetic field. These states are responsible for the anomalous integer quantum Hall effect [13–16], which had an important historical role in that it was the experimental result which drew the attention of the larger physics community as many considered it the smoking gun of relativistic Dirac electrons in graphene. The other effects, the parity anomaly and induced Chern–Simons terms, are less directly visible in graphene and have had to await the advent of topological insulators [17–20] to come into their own. This is by now well-worn ground, as evidenced by the excellent presentations at this symposium.

What I want to talk about today is another important subject, one of dynamics, the effects of the strong Coulomb interaction in graphene. This dynamics also has an analogue in relativistic quantum field theory, and in elementary particle physics, in the study of chiral symmetry breaking. The phenomenon of spontaneous chiral symmetry breaking is one of the cornerstones of our current understanding of strong nuclear interactions. The approximate chiral symmetry of almost massless quarks is spontaneously broken. Quarks gain mass and the Goldstone bosons are pions, which, because the symmetry is not exact, are light but not massless. It is a general view that this spontaneous symmetry breaking is driven by strong gauge field-mediated interactions, in the case of quantum chromodynamics, the exchange of gluons. It proceeds through the formation of a mass operator condensate, $\langle \bar{\psi} \psi \rangle$. This condensate breaks chiral symmetry, and fermion masses are the result. This phenomenon is important for strong interactions, but it could also be more far-reaching, as it is part of the circle of ideas behind some extensions of the standard model, technicolor models being an example.

Being a strong coupling phenomenon, chiral symmetry breaking is notoriously difficult to understand in a quantitative way. The standard quantum field theory tool of perturbation...
theory is not reliable in the strong coupling regime. One interesting way to gain intuition about chiral symmetry breaking has been to study the analogous phenomenon in simpler models, such as (2 + 1)-dimensional electrodynamics.

This toy model of chiral symmetry breaking \cite{21-28} is a (2 + 1)-dimensional quantum field theory with $U(N)$ symmetry:

$$L(x) = \frac{N}{4g^2} F_{\mu\nu}^2.$$ \hfill (1)

The minimal representation of the Dirac matrix algebra in three space–time dimensions is two—the fermions are a doublet spinor representation of the $SO(2, 1)$ Lorentz symmetry. Chirality symmetry in three space–time dimensions is intimately tied to symmetry under parity and time reversal. Generally, in any dimension, massless fermions have more symmetries than massive fermions. It is not possible to find a mass term $\sim \bar{\psi} \psi$ which has all of the symmetries of the kinetic term in the fermion Lagrangian, $i\bar{\psi} \gamma^{\mu} \partial_{\mu} \psi$. The kinetic terms in the three-dimensional (3D) fermion action are unaffected if we implement a parity transformation by making the replacement

$$\psi(x, y, t) \rightarrow \gamma^1 \psi(-x, y, t)$$ \hfill (2)

and change the integration variables accordingly. The kinetic term in the action

$$\int dt \, dx \, dy \, m \bar{\psi} \gamma^0 \psi$$ \hfill (3)

is invariant. However, a mass term, which is of the form

$$\int dt \, dx \, dy \, m \bar{\psi} \gamma^0 \psi,$$ \hfill (4)

changes sign under parity. One can formulate a parity invariant mass term if there is more than one species of fermions. For example, if there were two species and they had opposite signs of mass, so their mass terms were of the form

$$m \left[ \bar{\psi}_1 \psi_1 - \bar{\psi}_2 \psi_2 \right],$$ \hfill (5)

we could define a parity transformation by augmenting the transformation in (2) by an exchange of the two species,

$$\psi_1(x, y, t) \rightarrow \gamma^1 \psi_2(-x, y, t), \quad \psi_2(x, y, t) \rightarrow \gamma^1 \psi_1(-x, y, t).$$

The mass term (5) is invariant under this transformation, so parity is restored. On the other hand, the kinetic Lagrangian

$$\bar{\psi}_1 \gamma^{\mu} \partial_{\mu} \psi_1 + \bar{\psi}_2 \gamma^{\mu} \partial_{\mu} \psi_2$$

has a symmetry of exchanging $\psi_1 \leftrightarrow \psi_2$, which the mass term (5) does not have. This symmetry would actually be a larger continuous internal symmetry $U(2)$ or $O(2)$, depending on whether we are discussing complex Dirac fermions or charge-self-conjugate Majorana fermions.

If, on the other hand, we introduced the symmetric mass term,

$$M \left[ \bar{\psi}_1 \psi_1 + \bar{\psi}_2 \psi_2 \right],$$

it would break parity. There is no way to introduce a fermion mass without breaking either parity or some of the internal symmetry.

The above argument applies equally well if $\psi$ is a complex Dirac fermion or a charge-self-conjugate Majorana fermion. A complex fermion can be written as two Majorana fermions. Let us choose a specific representation for the Dirac matrices,

$$\gamma^0 = \sigma^2, \quad \gamma^1 = i \sigma^3, \quad \gamma^2 = i \sigma^1,$$

where $\sigma^a$ are Pauli matrices. With this convention, the Dirac equation

$$(i \gamma^\mu \partial_{\mu} + m) \psi = 0$$

is real, so it is satisfied by both $\psi$ and $\psi^*$, the complex conjugate. Then the complex fermion can be written as

$$\psi = \frac{1}{\sqrt{2}} \left( \psi_R + i \psi_I \right),$$

where $\psi_R = \psi^\dagger$ and $\psi_I = \psi^\star$, and we can write the action for a complex fermion as the sum of two actions, one for the real part and one for the imaginary part,

$$\frac{1}{2} \bar{\psi}_R \gamma^\mu \partial_{\mu} \psi_R + \frac{i}{2} \bar{\psi}_I \gamma^\mu \partial_{\mu} \psi_I.$$

We could introduce a parity invariant mass term for this system,

$$m \left[ \bar{\psi}_R \psi_R - \bar{\psi}_I \psi_I \right].$$

Note that this term can be non-zero, consistent with Fermi statistics. If $\psi_R = [\psi^\dagger]$, then $\frac{m}{2} \bar{\psi}_R \psi_R = m \, u \, v$ if $u$ and $v$ anticommute with each other. In terms of the original complex fermion, this mass term is

$$m \left[ \psi^\dagger \gamma^0 \psi + \psi \gamma^0 \psi^* \right],$$

which breaks the phase symmetry of the complex fermion. Such a mass term could appear in a superconducting state; for example, if superconductivity were induced in graphene using the proximity effect, it would be possible to have a relativistic mass term without breaking parity. In the following, we are going to always assume that the phase symmetry is not broken. In that case, we can limit the discussion to complex fermions. Then, if this phase symmetry is not broken, the possible mass terms for complex fermions must either break parity or what is generally an internal unitary symmetry. For example, graphene has emergent $U(4)$ symmetry. The phase symmetry corresponding to charge conservation, and which is a gauge to get electromagnetic interactions, is the $U(1)$ subgroup of $U(4)$. We are assuming that this subgroup survives in any chiral symmetry breaking scheme. The sort of symmetry breaking that we will consider will generally be

$$U(4) \rightarrow U(2) \times U(2) \text{ or } U(4) \rightarrow U(1)^4.$$

The quantum field theory (1) has a dimensional coupling constant, $g^2$. It is super-renormalizable in that all but a finite number of Feynman diagrams are ultraviolet divergent. However, perturbation theory in $g^2$ leads to severe infrared
differences [21]. Moreover, the low energy and momentum limit of the theory is strongly coupled. An alternative, renormalizable expansion can be carried out using the dimensionless parameter \( \frac{1}{N} \) [22]. The theory is solvable in the large \( N \) limit, that is, when the number of fermion species \( N \) is taken to infinity, and there is a systematic expansion in \( \frac{1}{N} \). However, in the large \( N \) limit, the interaction is of order \( \frac{1}{N} \) and it is too weak to break chiral symmetry. It is thought that, as \( N \) is lowered to smaller values, and the interaction gets stronger, it eventually reaches a critical value after which chiral symmetry is broken. Estimates of critical \( N \) vary from 1.5 to 4.5, the spread being a symptom of the lack of accuracy of perturbative computations in loop integrals for quantities such as the polarization tensor given by the non-local term in the action. In (6), it was fixed by the number of fermions that were integrated out, whereas in (7) it is determined by the dielectric constant of the medium in which graphene is immersed.

Although the graphene model (7) is nonrelativistic, our discussion of chiral symmetry breaking applies to it as well as the relativistic theory. A mass term for the fermion would break either parity symmetry or some of the emergent \( U(4) \) symmetry. In fact, at the lattice level, the relevant parts of the \( U(4) \) symmetry are replaced by sublattice symmetry—the symmetry of the graphene Hamiltonian when interchanging the two triangular lattices that make up the honeycomb lattice. Breaking this symmetry is intimately related to forming a gap in the fermion spectrum [1].

The nonrelativistic field theory with action (7) is a renormalizable quantum field theory, in the sense that, in perturbation theory in its dimensionless coupling constant \( e^2 \), no new counterterms have to be introduced to cancel ultraviolet divergences [42–56]. This has been confirmed explicitly up to order two loops. Renormalizing perturbation theory requires a logarithmically divergent counterterm for \( v_F \), which then becomes a scale-dependent parameter, running to larger values in the infrared limit. The perturbative beta function vanishes at the Lorentz invariant limit, \( v_F = c \). It is conjectured that the coupling constant \( e^2 \) remains a tunable parameter, so that the theory has a fixed line where it would be a conformal field theory with a tuneable constant \( e^2 \). However, if one uses the one-loop beta function, and the known value of \( v_F \) at the lattice scale as a boundary condition, \( v_F \) runs so slowly that to even get to the order of \( c/10 \) requires wavelengths of the magnitude of meters, larger than the length scales achievable in experiments. Moreover, the graphene fine structure constant, which controls loop corrections in perturbation theory, is large:

\[
\alpha_p \equiv \frac{e^2}{4\pi \hbar v_F} = \frac{e^2}{4\pi \hbar c v_F} \approx \frac{300}{137}.
\]

This is the constant which occurs in loop integrals for quantities such as the polarization tensor given by the Feynman diagram in figure 1.

If the effective coupling constant is really this large, the accuracy of perturbative computations is questionable at best.

The central question which we shall address in the following is: given that the Coulomb interaction is strongly coupled, is the interaction strong enough to break chiral symmetry? Part of the question is as to whether, if the coupling were variable, there is a critical value of the coupling where a quantum phase transition occurs, particularly to a
phase where chiral symmetry is broken. The second question is as to whether the physical parameters of graphene put it in or close to this range. The current experimental status of graphene, where there is no evidence of spontaneous gap formation, at least in the absence of strong magnetic fields [57–61], suggests that the answer to the second question is no. If there would be a quantum phase transition, the coupling in real graphene is apparently not strong enough. The fact that it could be close to being strong enough is also tantalizing, as some mechanical or other physical deformation of graphene could then make it closer, and drive it to the phase transition. We will spend the next section on an attempt to understand why the strong coupling in graphene might be strong enough and why it might be close, but we do not as yet have a quantitative estimate of how close.

We should mention that this idea has been pursued in some lattice simulations [29–38]. It has also been addressed using a lattice strong coupling expansion [39]. These studies do not use the graphene lattice, but a square lattice with magnetic flux to produce relativistic fermions. They seem to answer the question as to whether chiral symmetry breaking would exist in the affirmative. One uncertainty that remains is whether the same results would hold for a honeycomb lattice. One might expect universal features such as critical exponents to be predictable; however, the non-universal details such as the value of critical couplings could differ.

Finally, there is a large $N$ expansion which indicates that sufficiently strong contact interactions could drive chiral symmetry breaking. This fact has been known for a long time in the particle physics literature and it is exploited for the physics of graphene in [40, 41, 53–56]. In [40, 41], they find that the local on-site interactions are crucial and that the Coulomb interaction makes only a weak modification of the critical behavior, which is essentially driven by the point interactions. This is not much different from what we shall find.

Before we proceed, we should mention another idea that has been pursued recently: the use of string theory holography to study the strong coupling limit of field theories, which could be regarded as deformations of graphene. Interestingly, using holography, it is possible to construct two different scenarios [62, 63]. In one [62], there is a strong coupling fixed point for the analogue of $\epsilon^2$ where chiral symmetry is broken if $\epsilon^2$ is sufficiently large, and the mass gap is small only if $\epsilon^2$ is tuned to be sufficiently close to this fixed point. In the other construction [63], $\epsilon^2$ is tunable all the way to infinity and there is no phase transition. Instead the theory is a non-trivial conformal field theory and chiral symmetry is only broken after turning on a dangerous relevant operator, related to the mass operator. Interestingly, the first scenario, where the field theory inhabits a planar defect in a single $(3+1)$-dimensional gauge theory and where there is a chiral phase transition, bears a certain resemblance to suspended graphene, whereas the second scenario, where the field theory inhabits a planar boundary between two different gauge theories, has a similarity to graphene on a substrate.

2. Strong coupling expansion

If the graphene fine structure constant is really as large as the estimate in (8) perturbation theory is of no use in analyzing the effects of the Coulomb interaction. The alternative of a strong coupling expansion would be the more reasonable approach. Strong coupling expansions of relativistic gauge field theories, once they are regulated by putting them on a lattice, give a nice qualitative picture of confinement. However, they are far from the continuum limit and are notoriously non-universal, particularly for questions involving chiral symmetry breaking, where different definitions of the lattice theory that have the same naive continuum limit can have wildly different results. However, graphene comes from a lattice to begin with. One could begin with a reasonable estimate of the lattice Hamiltonian of graphene as the starting point for a strong coupling expansion.

We will assume that graphene is modeled by the following Hamiltonian:

$$H = H_e + H_c,$$

where the hopping term is

$$H_e = t \sum_{\alpha, \sigma} \left( \psi_{\alpha, \sigma} \psi_{\alpha, \sigma} + \psi_{\alpha, \sigma}^\dagger \psi_{\alpha, \sigma} \right)$$

and the Coulomb interaction is

$$H_c = \frac{e^2}{8\pi} \sum_n u_n \rho_n^2 + \frac{e^2}{8\pi} \sum_{\sigma \neq \sigma} \frac{1}{|n - n'|} \rho_n \rho_{n'}. \tag{11}$$

The electron creation and annihilation operators are denoted by $\psi_{\sigma, \alpha}$ and $\psi_{\sigma, \alpha}^\dagger$. They have spin label $\sigma$ with two spin states $\sigma = \uparrow$ and $\sigma = \downarrow$, and site label $n$, which can be on either the sublattice A or B. The non-vanishing anticommutators are

$$\{\psi_{\sigma, n}; \psi_{\sigma', n'}^\dagger\} = \delta_{n'n} \delta_{\sigma \sigma'}.$$ \tag{12}

The space of quantum states is a Hilbert space constructed by cyclic action of creation operators on the empty ‘vacuum’ state, $|0\rangle$, which obeys $\psi_{\sigma, n}|0\rangle = 0$ for all values of the labels $\sigma$ and $n$.\(^1\) We will consider the case where the graphene sample is neutral, that is, half of the available electronic states are occupied. The electron density operator in (11) is given by

$$\rho_n = \psi_{\uparrow, n}^\dagger \psi_{\uparrow, n} + \psi_{\downarrow, n}^\dagger \psi_{\downarrow, n} - 1.$$ \tag{13}

The ‘$-1$’ in the density represents the positive ion which occupies each site of the lattice. The spectrum of the electron charge operator $\psi_{\uparrow, n}^\dagger \psi_{\uparrow, n}$ is $0, 1, 1, 2$ and the spectrum of $\rho_n$ is $-1, 0, 1, 2$, according to whether the site is unoccupied, singly occupied or doubly occupied, respectively. Double occupation is allowed by Fermi statistics because there are two spin states.

$H_e$ describes the energy due to tunneling between tight-binding states on adjacent lattice sites. A labels a point on sublattice A and the points $A + \alpha$ are on sublattice B. The lattice is depicted in figure 2. It is the continuum limit of $H_i$ which produces the Dirac Hamiltonian which is used for the description of electron dynamics close to the Fermi level in graphene. The hopping amplitude in $H_i$ has the approximate magnitude $t \sim 2.7 eV$.

\(^1\) We are ignoring subtleties of exactly how this Hilbert space would be defined in a system with infinite volume.
obtained in the continuum limit of $H_f$ when the system is charge neutral. This sort of mass term is invariant under time reversal and parity, but it breaks some of the emergent $U(4)$ symmetry of the continuum limit. If both parameters $\mu_0$ and $|\tilde{\mu}|$ are nonzero, the symmetry-breaking pattern is $U(4) \to U(1)^4$. If either $\mu_0$ or $|\tilde{\mu}|$ is zero, but the other nonzero, the pattern is $U(4) \to U(2) \times U(2)$. For the most part, it is the latter symmetry breaking pattern that we shall discuss in the following. At this point, we should note that there are other kinds of symmetry breaking which are possible. These have to do with distortions of the graphene lattice which lead to bond order, like the Kekulé distortion. That sort of symmetry breaking is analogous to the Peierls instability of 1D tight-binding models and it is an important possibility for graphene and some of the interesting consequences have been pursued in a number of works [65–67].

Our goal is to find the ground state of the full Hamiltonian in (9). We are not able to find an exact solution. We therefore have to resort to an approximation. Since, as we have argued above, the Coulomb energy is typically larger than the kinetic energy of electrons, we will begin by seeking a ground state of the Coulomb Hamiltonian, $H_c$.

To do this, we first observe that the charge density operators are Hermitian and, at different sites, they commute with each other,

$$[\rho_n, \rho_{n'}] = 0.$$  \hspace{1cm} (16)

Thus, the charge densities and therefore also the Coulomb Hamiltonian $H_c$ can be simultaneously diagonal. This fact effectively makes finding the lowest energy state of $H_c$ a classical problem—we need only find that classical distribution of unit point charges which minimizes the Coulomb energy. If we consider the Fourier transform of the charge density

$$\rho_n = \int_{\Omega_B} \frac{d^2k}{\sqrt{2\pi a}} e^{i k \cdot n} \hat{\rho}(k),$$  \hspace{1cm} (17)

where $\Omega_B$ is the Brillouin zone of the triangular A sublattice. The Coulomb energy is diagonal in charge densities,

$$H_c = \frac{e^2}{4\pi \epsilon a} \int d^2k \left| \hat{\rho}(k) \right|^2 \left( \frac{\mu_0}{2} + \sum_{n \neq 0, n \in A} e^{i k \cdot n} \left[ \frac{1}{|n|} + \frac{\cos k \cdot s_i}{|n + s_i|} \right] \right).$$  \hspace{1cm} (18)

The absolute minimum is where $\hat{\rho}(k) = 0$. This is compatible with the precisely half-filled lattice that we are considering since the constraint of half-filling is $\hat{\rho}(0) = 0$. This is the completely neutral state. This neutral state has one electron occupying each lattice site, as in figure 3.

However, we are not finished yet. This is a highly degenerate state, as each electron has either spin polarization, up or down. The state itself is

$$|\sigma_n\rangle = \prod_n \psi_{\sigma, n} |0\rangle,$$  \hspace{1cm} (19)

where $\sigma_n$ is the spin orientation at site $n$. The degeneracy of this state is $2^V$, where $V$ is the total number of sites. All of

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{The honeycomb graphene lattice with sublattices A and B depicted by black and white dots, respectively. The sublattices are connected by $s_i$.}
\end{figure}
these states are insulators. The linear combination of them that becomes the preferred ground state will also be an insulator. The spectrum of the electron has a mass gap.

As usual, this degeneracy must be resolved in perturbation theory by including perturbations from the kinetic Hamiltonian $H_t$. The states are mixed at second order in perturbation theory, where $H_t$ can implement transport from a site to a neighbor and then back again. When the process is allowed, second-order perturbation theory always lowers the ground state energy. Here, it is allowed when the spin orientation of neighbors is opposite. The result is that the lower energy state is an antiferromagnet. To see this in technical terms, the effective Hamiltonian for the degenerate ground states is

$$H_{\text{eff}} = -H_t \frac{1}{H_e} H_t$$

$$= -\frac{e^2}{4\pi\epsilon_0} (u_0 - 1) \sum_{A,\sigma,\sigma'} \left( \psi_{\sigma, A} \psi_{\sigma', A} + \psi_{\sigma, A} \psi_{\sigma', A}^\dagger \right)$$

Using the sum rule for Pauli matrices

$$\tilde{\sigma}_{\sigma\sigma'} \cdot \tilde{\sigma}_{\sigma'\sigma''} = 2\delta_{\sigma\sigma'} - \delta_{\sigma\sigma'} \delta_{\sigma\sigma''},$$

we can write the effective Hamiltonian as

$$H_{\text{eff}} = \frac{e^2}{4\pi\epsilon_0} (u_0 - 1) \sum_{A,\sigma} \left( \psi_{\sigma, A} \psi_{\sigma, A}^\dagger \right)$$

which is the Hamiltonian of the quantum Heisenberg antiferromagnet with nearest-neighbor coupling. We have dropped terms containing the charge density, as all states that this Hamiltonian would act on are eigenstates of charge density with zero eigenvalue. The magnitude of the coefficient in front of the Hamiltonian is 1 eV, which sets the scale of both the ground state energy and the energy of excitations.

Figure 3. The lowest energy state of the Coulomb interaction has one electron localized at each site. This is a highly degenerate state as the spins of the electrons are arbitrary.

Figure 4. The elementary excitation of the lattice with one electron at each site. The energy of this state is denoted by $U$ and is of the order of 10 eV.

of the antiferromagnet. The ground state of the Hamiltonian in (22) is known to be an antiferromagnetically ordered state which breaks the sublattice symmetry. The classical approximation to the ground state of the antiferromagnet with order parameter oriented along the $z$-axis is

$$|\text{afm}\rangle = \prod_{A} \psi_{1, A}^\dagger \prod_{B} \psi_{1, B}^\dagger |0\rangle.$$  

In $H_e$ in equation (15), the second term would have nonzero expectation value. The magnitude of this expectation value is somewhat smaller than the coefficient of the effective Hamiltonian in (22).

The Coulomb ground state that we have come up with is identical to the ground state of the half-filled Hubbard model. In addition, the lowest energy charged excitation, depicted in figure 4, is also identical to the lowest energy charged excitation of the half-filled Hubbard model. To describe it and its very low energy dynamics, it is tempting to replace the Coulomb Hamiltonian by the Hubbard model whose Hamiltonian is

$$H = I \sum_{A,\sigma} \left( \psi_{\sigma, A}^\dagger \psi_{\sigma, A} + \psi_{\sigma, A} \psi_{\sigma, A}^\dagger \right)$$

$$+ \frac{U}{2} \sum_{\sigma,\sigma',\sigma''} \left( \sum_{\sigma'} \psi_{\sigma, A}^\dagger \psi_{\sigma', A} \psi_{\sigma, A} \psi_{\sigma', A}^\dagger - 1 \right)^2,$$

where $U = \frac{e^2}{4\pi\epsilon_0} (u_0 - 1)$ is the energy of the state in figure 4. The Hubbard model is short-ranged. It simply penalizes non-single occupation of sites, in the large $U$ limit, projecting onto singly occupied sites. Note that the Coulomb Hamiltonian is a little stronger than the Hubbard one in that, for Hubbard the energy of the lowest excitation—the electron–hole pair—is independent of the distance between them, whereas for Coulomb, they have opposite charge and would still attract and would tend to fall together. This should make the ground state that we are discussing more stable.
for the Coulomb Hamiltonian than for the Hubbard model. It might therefore have a higher critical coupling.

The Hubbard model (24) and the Heisenberg antiferromagnet on a honeycomb lattice have been studied both by analytic and numerical techniques [68–72]. It is known that in the limit where \( U/t \to \infty \), the ground state has antiferromagnetic order. This is the chiral symmetry breaking state. Our mapping of the Coulomb interaction at half-filling onto this class of models would then seem to answer in the affirmative the question as to whether a strong enough Coulomb interaction would break chiral symmetry.

Indeed, we have thus argued that, when the Coulomb interaction is dominant, the ground state is a spin density wave, which gives rise to a chiral symmetry breaking mass term in the Hamiltonian of the type (15) and the chiral symmetry is broken as \( U(4) \to U(2) \times U(2) \). It is also clear from the numerical studies that when the parameter \( U/t \) is small, the hopping dominates the Hubbard model and the system is in a metallic phase, which is the one described by the tight-binding model of graphene. In [69], the phase transition between these two regimes is estimated to be in the range

\[
4 \leq \frac{U}{\tau_{\text{crit}}} \leq 5.
\]

This is very interesting as a rough estimate of this parameter in graphene, \( \frac{U}{\tau} \sim 2–4 \), puts it in a regime that is just sub-critical. It is a tantalizing idea that, if graphene could be modified in some way, perhaps mechanically by stretching it, to increase \( U/t \), this process could drive a quantum phase transition which would result in chiral symmetry breaking.

Even more intriguing is a recent Monte Carlo study of the Hubbard model on a honeycomb lattice which finds an intermediate phase in the region

\[
3.5 \leq \frac{U}{\tau} \leq 4.3,
\]

which appears to be resonating valence bond spin liquid [70]. What such a phase would mean for graphene has not been explored yet. We note that we expect that the Mott insulator phase of graphene is well modeled by the Hubbard model. Beyond the first phase transition, the long-ranged fields of the Coulomb interaction could well take over and the spin-liquid to metal phase transition might not be accurately described by the Hubbard model.

In a certain sense, we have answered the question as to why such a strong Coulomb interaction does not break chiral symmetry in graphene. Even if the coupling is very strong, the first pass at the strong coupling ground state has a uniform charge distribution, no charge density wave and no chiral symmetry breaking. We then need to rely on a subtle effect from degenerate perturbation theory to make the system an antiferromagnet. In fact, the energy scale of the antiferromagnet is \( r^2/U \), which is smaller if the coupling \( U \) is larger. Put simply, chiral symmetry breaking is charge density wave formation and a strong Coulomb interaction favors a homogeneous neutral state over a charge density wave. We must then rely on more subtle effects to create a spin density wave which is charge neutral.

3. Spinless electrons

To see how results could have been different, consider the case of a half-filled graphene lattice where the electron has one rather than two spin states. In this case, the density of neutral graphene would have one half of the sites of the lattice occupied. The \(-1\) in the charge density in (13) is replaced by \(-\frac{1}{2}\) —if the neutral system is to be half-filled, the positive ion residing on each site must have charge \( -\frac{1}{2} \). Thus, the eigenvalues of the charge density at a site are never zero—the eigenvalues of \( \rho_n \) would be \( \pm \frac{1}{2} \), depending on whether the site is occupied or unoccupied. This means that there is no charge neutral state. Having no possibility of a neutral state, the electrons do the next best thing; they maximize the effect of electron–hole attraction, which contributes negatively to the energy and is strongest if the electron and the hole are on nearest-neighboring sites. The Coulomb energy is minimized by the Wigner lattice that is depicted in figure 5. This state has the same on-site Coulomb energy as any other state (since \( \rho^2_n = 1/4 \)) and every set of nearest neighbors which have opposite charges and contribute \( -\frac{e^2}{4a} \) to the energy, where \( a \) is the lattice spacing.

Since this state has all of the electrons residing on one of the sublattices, it immediately breaks chiral symmetry in the maximal possible way. The hopping term in the Hamiltonian would have to be very large to restore translation invariance and the metallic state in this system. Surely, one-spin-state graphene with other parameters similar would be an insulator.

It is interesting that there is such a difference between the two cases, spinful graphene and spinless graphene. One would be gapless, and the other would be gapped and would be a strong insulator. In the low energy limit, the only difference between the two is the \( U(4) \) versus \( U(2) \) symmetry. It is an open question as to whether one can discern the difference of critical couplings at the level of continuum field theory.

Figure 5. The charge distribution of the strong coupling ground state of neutral graphene with a single spin is a Wigner crystal where one of the sublattices is completely occupied and the other sublattice is completely empty.
4. Discussion

Coming back to graphene with spin, we observe that, almost for accidental reasons, the most important part of the Coulomb interaction was the short-ranged on-site interaction. The relevance of the short-ranged part of the electromagnetic interactions is consistent with renormalization group arguments which show that local four-Fermi interactions dominate the chiral symmetry breaking quantum phase transition [49]. The renormalization group flow, computed in the $2+\epsilon$ expansion in [49], is depicted in figure 6. It shows the Gross–Neveu fixed point which dominates the renormalization group flow when the local point interaction coupling of the Gross–Neveu model (plotted on the horizontal axis) is critical. When the electromagnetic interaction (plotted on the vertical axis) is turned on, it lowers the critical coupling somewhat.

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