Interaction driven metal-insulator transition in strained graphene

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The question of whether electron-electron interactions can drive a metal to insulator transition in graphene under realistic experimental conditions is addressed. Using three representative methods to calculate the effective long-range Coulomb interaction between π-electrons in graphene and solving for the ground state using quantum Monte Carlo methods, we argue that without strain, graphene remains metallic and changing the substrate from SiO₂ to suspended samples hardly makes any difference. In contrast, applying a rather large – but experimentally realistic – uniform and isotropic strain of about 15% seems to be a promising route to making graphene an antiferromagnetic Mott insulator.

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Over the past decade graphene has established itself as a remarkable new material with superlative properties [1,2]. However, the early hopes to utilize it as a next generation transistor have been dashed mostly because graphene remains metallic – these prototypical Dirac fermions are immune to many of the conventional routes for driving two-dimensional electron gases into an insulating state, including, for example, Anderson localization and percolation transitions (see e.g. Ref. [3]). Other mechanisms for opening band-gaps including hydrogenation [4], application of uniaxial strain [5] and forming nanoribbons [6] severely degrade graphene’s mobility. Very recently, moiré heterostructures using graphene and hexagonal boron nitride have shown evidence of an insulating phase [7,8], although interpreting these results remains somewhat controversial [9,12].

In this Letter, we explore a different avenue to make graphene insulating, namely, utilizing the electron-electron interactions. Despite much study on the effects of interactions in graphene [13] it is surprising how much still remains to be understood. While it is clear that without any electron-electron interactions, graphene should be a semi-metal (SM), and that for very strong interactions it should be an insulating anti-ferromagnet (AFM), it remains unclear what one should expect for the real graphene material. For example, there are distinct claims in the literature that suspended graphene should be insulating, strongly metallic and weakly metallic [13-16]. This discussion could have practical relevance as it could be the basis for a low power Mott-transistor [17].

In this work we explore different ways of controlling the effective strength of electron-electron interactions in realistic graphene devices, and propose how one can move around its phase diagram. In particular (and in contrast to what is widely assumed to be true [2,13]), we demonstrate that it is the non-universal, material-specific and short-range part of the electron-electron interactions that plays the dominant role in determining graphene’s ground state. More interestingly, we conclude that application of isotropic strain is considerably more efficient in approaching the SM-AFM phase transition than substrate manipulation, providing a new route for driving the system into the elusive Mott insulating phase that has yet to be observed experimentally.

The Hubbard model has served as a versatile paradigm to study interacting electrons on a lattice. It is defined as an effective model for electrons in partially filled narrow energy bands of a crystal’s spectrum. While the canonical Hubbard model includes only on-site interactions, the effects of longer range interactions are incorporated by a straightforward generalization of the two-body interaction term, described by the Hamiltonian

\begin{equation}
\hat{H} = -t \sum_{\langle ij \rangle, \sigma} (\hat{c}^\dagger_{i \sigma} \hat{c}_{j \sigma} + \text{h.c.}) + \sum_i \hat{n}_{i \uparrow} \mathcal{V}_i \hat{n}_{i \downarrow} + \frac{U}{2} \sum_{i \neq j} \sum_{\sigma, \sigma'} \hat{n}_{i \sigma} \mathcal{V}_{ij} \hat{n}_{j \sigma'},
\end{equation}

where \( \hat{c}_{i \sigma} \) (\( \hat{c}_{i \sigma}^\dagger \)) creates (annihilates) an electron of spin \( \sigma = \uparrow, \downarrow \) at position \( r_i \), while \( \hat{n}_{i \sigma} = \hat{c}_{i \sigma}^\dagger \hat{c}_{i \sigma} \) gives the density of electrons with spin \( \sigma \) at position \( r_i \). The nearest neighbor hopping integral is identified by \( t \), while \( \mathcal{V}_{ij} \) stands for the interaction between electrons at sites \( i \) and \( j \). We note that a realistic description of graphene requires the parameters \( \mathcal{V}_{ij} \) to be fixed in accordance with the spatial profile of the (partially screened) Coulomb interaction \( \mathcal{V}(r) \) that results from the screening of the bare Coulomb interaction by electrons in energy bands other than the \( \pi \)-bands.

It is well established that the canonical Hubbard model
three representative methods to capture the full spatial
dependence of the system, yet their real values are unknown. We use
effective approximations. For instance, we obtain
the value of the Coulomb potential between electrons at
half-filling, an experimentally feasible amount of strain
would drive graphene into an interaction driven insulating
phase, which could be then measured in compressibility,
transport or scanning probe experiments.

However, ignoring longer range interactions in
graphene is problematic since the long-range tails of the
Coulomb potential between Dirac fermions cannot be ef-
ciently screened. To address these Coulomb tails,
it was recently conjectured that the effects of non-
local interactions can be mapped into the Hubbard model
with an on-site interaction parameter $U$ for realistic experimental realizations of
graphene vary widely in the literature, with values ranging from $U \approx 1$ eV to 10 eV (where the lower estimates would suggest that graphene is metallic, while the higher estimates hint at it being insulating).

Here we study the possibility to drive graphene across
the SM-AFM phase transition by substrate manipulation
or application of biaxial (i.e. uniform and isotropic)
strain – see Fig. 1. First we must fix the long-range
Hubbard model’s parameters $V_{ij}$. These are the crucial ingredients determining the ground state properties of the system, yet their real values are unknown. We use three representative methods to capture the full spatial
profile of the partially screened Coulomb interaction for
$p_z$ electrons in realistic graphene, and choose $V_{ij}$ accordingly. These methods will be discussed in detail below, but now we just introduce their names: Thomas-Fermi (TF), constrained random phase approximation (cRPA) and the quantum chemistry – Pariser-Parr-Pople (QC-PPP) method. We then investigate the effect of biaxial strain and substrate manipulation on the partially
screened Coulomb potential $V(r)$. We find (see Fig. 2)
that biaxial strain strongly modifies the $V(r)$ close to
$r = 0$ (not affecting the long-range interactions), while
changing the substrate (which changes both the dielectric screening and the amount of disorder) only weakly modifies the long-range tail of $V(r)$. Finally, using
quantum Monte Carlo techniques (finite temperature deter-
minant quantum Monte-Carlo and zero-temperature pro-
jective quantum Monte-Carlo), we simulate the ground
state of the long-range half-filled Hubbard model (in the
honeycomb lattice) with the $V_{ij}$ obtained from $V(r)$, and
argue that at least within the Thomas-Fermi approxima-
that the Coulomb interaction felt by the $p_z$ electrons is given by
$V(r) = [1 - V_{\text{bare}}(r)]P_z^{-1}V_{\text{bare}}(r)$, where $V_{\text{bare}}(r)$ stands
for the bare Coulomb potential. The accuracy of this
method has long been debated in the literature (see e.g. Ref. [32]), and its results are often difficult to interpret
physically. For graphene, the fact that the Dirac band
spans a broad energy window further complicates the ap-
plication of the cRPA formalism. Notwithstanding these
difficulties, the cRPA remains the best numerical tech-
ique at our disposal to determine the $V_{ij}$ for graphene.
In this manuscript we use the cRPA results previously
obtained in Ref. [25], which compute $U$, $V$ and $t$ for bi-
axial strains up to 12%. In this range of strains all these
parameters show a linear behavior. In order to obtain
the cRPA values of $U$, $V$ and $t$ for up to 18% strain (see Fig. 2a) we have assumed that this linear behavior re-
ains unchanged, extracting $U$, $V$ and $t$ from a linear fit
to Ref. [25]’s numerical results.

The QC-PPP method (see e.g. Vérégés et al. [53])
works by using ab initio Hartree-Fock and post-Hartree-
Electrons positioned at neighboring atoms (distance $\delta$) while the Coulomb interaction between two $\pi$-bands’ electrons positioned at neighboring atoms (distance $\delta$) is given by

$$ V = \frac{e^2}{4\pi \epsilon} \int d^3 r_1 d^3 r_2 \left| \phi(r_1 + \delta) \right|^2 \frac{e^{-k_0 |r_1 - r_2|}}{|r_1 - r_2|} \left| \phi(r_2) \right|^2. \tag{3} $$

Here, $\phi(r)$ stands for the $p_\pi$-orbital’s wave-function which we approximate by that of atomic hydrogen. The free parameter $k_0$ in Eqs. (2) and (3) is fixed by requiring that the hopping integral

$$ t = \int d^3 r \phi^*(r + \delta) \left[ -\frac{\hbar^2 \nabla^2}{2m} + \frac{e^2}{4\pi \epsilon} \sum_i e^{-k_0 |r - R_i|} \right] \phi(r), \tag{4} $$

is equal to the literature accepted value of $t_0 = 2.7$ eV [21]. In parallel with what we do for the other two methods, we then interpolate between $V_{ij}$’s short-range values $U$ and $V$ and the long-range tail of $V_{ij}$ (see below). The procedure used to compute $V_{ij}$ of biaxially strained graphene is similar to that discussed earlier [34].

The computationally demanding method employed prevents us from simulating large size systems. In particular, one must include the effect of the surrounding electrons since their inter-band polarizability contributes at all length scales [21] thus modifying the effective dielectric constant from $1/r$ to $1/[r(1 + \pi r/s)]$, where $r_s = 2e^2/[(\kappa_a + \kappa_b) \hbar v_F]$, $s$ is the effective fine structure constant (where $\kappa_a$ and $\kappa_b$ are the dielectric constants above and below the graphene flake). The presence of disorder in the substrate can also be accounted for by introducing a modified screening function (see e.g. Ref. [35]).

The full profile of the partially screened Coulomb interaction

![Effect of biaxial strain](image1)

**FIG. 2.** Effect of biaxial strain (left panel) and substrate (right panel) on the partially screened Coulomb interaction. We use three representative models: constrained Random Phase Approximation (cRPA), circles/full curves; quantum chemistry – Pariser-Parr-Pople (QC-PPP), squares/dashed curves; and Thomas-Fermi (TF), triangles/dot-dashed curves. (a) Suspended graphene both unstrained and subject to 18% biaxial strain. (b) Unstrained graphene both suspended and deposited on SiO$_2$ compared to the bare Coulomb potential.

Fock techniques to solve for the ground state energy of molecules comprising a small number of benzene rings. These energies are then compared to an exact diagonalization of the long range Hubbard model where the Ohno interpolation formula, $V(r) = U/\sqrt{1 + (Ur/e)^2}$, is assumed for the Coulomb interaction. The $V(0) = U$ is a free parameter that is fixed by requiring the minimization of the root-mean square of the ground state energy of the $ab$ initio calculations and that of the long range Hubbard model. The QC-PPP values of $U$ and $V$ used in this manuscript were extracted from Ref. [33], which calculates $V(r)$ for the phenalenyl (3H-C$_{13}$H$_9$) molecule. This method gives an upper bound for the Hubbard $U$ in graphene since larger molecules would have more screening and reduced $V(r)$. Both the validity of the Ohno inter-polarization and the extrapolation to larger size systems give some reasons for caution. It has nonetheless proven extremely useful for small $\pi$-conjugated planar polycyclic aromatic hydrocarbons comprising tens of atoms such as anthracene and polyacenes [33, 34].

Finally, inspired by the work of Jung and MacDonald [26] we have constructed a Thomas-Fermi model to account for the screening of higher energy bands in graphene. Within the Thomas-Fermi screening approximation the on-site interaction $U$ is given by

$$ U = \frac{e^2}{4\pi \epsilon} \int d^3 r_1 d^3 r_2 \left| \phi(r_1) \right|^2 \frac{e^{-k_0 |r_1 - r_2|}}{|r_1 - r_2|} \left| \phi(r_2) \right|^2, \tag{2} $$

while the Coulomb interaction between two $\pi$-bands’ electrons positioned at neighboring atoms (distance $\delta$)
is obtained by interpolating between the short-range results, at first neighbor distance, and the long-range tail (assumed to start at the fourth neighbor).

As we can see in Fig. 2, the short-range part of the partially screened Coulomb interactions $\mathcal{V}(r)$ is strongly affected by biaxial strain (left panel), while its long-range tails are nearly insensitive to strain. Manipulating the substrate has a very weak effect on the long-range tails of the partially screened Coulomb interactions (right panel).

With the electron-electron interaction profiles of Fig. 2 we have fixed the long range Hubbard model’s parameters $\mathcal{V}_{ij}$ and explored its ground state using auxiliary field quantum Monte Carlo simulations (made possible by recent works [18, 36, 37]) – a numerically exact method for investigating strongly correlated systems. In this manuscript, we use different implementations of the auxiliary field quantum Monte Carlo technique: finite temperature determinant quantum Monte Carlo (DQMC), temperature projective quantum Monte-Carlo (PQMC), and zero-temperature determinant quantum Monte Carlo technique: finite temperature quantum Monte Carlo since its partially screened Coulomb interactions are non-local interaction comparable with the off-diagonal matrix elements associated with the non-local interactions, which renders the off-diagonal matrix elements associated with the long-range Hubbard model’s parameters $\mathcal{V}_{ij}$ insensitive to strain (left panel).

In particular, we find that the transformation matrix corresponding in the atom of sub-lattice $A, B$ is obtained from the QC-PPP model (we refer the reader to Ref. [38] for details); and zero-temperature projective quantum Monte-Carlo (PQMC) (for details see e.g. Ref. [39]), where the correlation functions are given by

$$
\langle \hat{O} \rangle = \frac{1}{Z} \sum \mathcal{D}[\phi_i, \phi_j] e^{-\beta \mathcal{H}[\phi_i, \phi_j]} \langle \hat{O}[\phi_i, \phi_j] \rangle
$$

(we refer the reader to Ref. [38] for details); and finite temperature projective quantum Monte-Carlo (PQMC) (for details see e.g. Ref. [39]), where the correlation functions are given by

$$
\langle \hat{O} \rangle = \frac{\langle \Phi_0 | \hat{O} | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} = \lim_{\beta \to \infty} \langle \Psi_T | e^{-\beta \mathcal{H}/2} \hat{O} e^{-\beta \mathcal{H}/2} | \Psi_T \rangle
$$

(6)

In both cases we use a Hubbard-Stratonovich transformation to convert the interaction term into a non-interacting term coupled to an auxiliary field. This transformation enables us to treat Hubbard models with non-local electron interactions, provided that the long-range interaction gives rise to a transformation matrix that is positive definite (a non-positive definite transformation matrix corresponds to a diverging auxiliary field).

In particular, we find that the transformation matrix for the case where the $\mathcal{V}_{ij}$ is obtained from the QC-PPP model is not positive definite. This is a direct consequence of the interpolation scheme mentioned above, which renders the off-diagonal matrix elements associated with the non-local interaction comparable with the diagonal elements associated with the local interactions. As a result, we could not use quantum Monte Carlo to simulate the quantum-Peierls-Pool model as an inhomogeneous system, leading to a diverging auxiliary field.

In the DQMC, we used inverse temperature $\beta = \frac{1}{T}$ in Eq. 5 between 24 and 36, which is sufficient to probe the low-energy behavior of the system. In the PQMC, we chose the Hartree-Fock state as our trial wave-function, $|\Psi_T\rangle$, using $\Theta t = 40$ (see Eq. 5) to project the wave-function onto the ground state. We made use of the scaling behavior of the antiferromagnetic structure factor ($S_{AFM}$) to estimate the magnetic state of the system.

$$
S_{AFM} = \frac{1}{L^2} \sum_{i,j} \left[ \langle m_i A m_j A \rangle + \langle m_i B m_j B \rangle \right],
$$

where $m_i C$ stands for the magnetization of the site located in the atom of sub-lattice $A, B$ of the unit cell $r_i$, while $L^2$ is the number of unit cells (i.e. $N = 2L^2$ sites). The system’s AFM order parameter is given by $m_{AFM} = \sqrt{S_{AFM}(2L^2)}$ (on top) and scaled antiferromagnetic structure factor $S_{AFM}(2\beta/\nu)/N$ (bottom) in terms of the inverse system size. We have used both projective quantum Monte Carlo (blue) and determinant quantum Monte Carlo (red) to study the phase of graphene subject to: 18% biaxial strain within the Thomas-Fermi model (upper points); 18% biaxial strain within the constrained RPA model (middle points); 0% strain within both the Thomas-Fermi and the constrained RPA models (lower points). We could not simulate the quantum chemistry – Pariser-Parr-Pople model with auxiliary field quantum Monte Carlo since its partially screened Coulomb potential gives rise to diverging auxiliary fields.

Figure 3 shows the dependence of $m_{AFM}$ and $S_{AFM}$ with the system size. For unstrained graphene both the cRPA and TF methods show $S_{AFM}$ decreasing with system size (and $m_{AFM}$ extrapolating to zero in the thermodynamic limit $L \to \infty$), indicating that without strain suspended graphene is metallic (in agreement with experimental observations). However, most interestingly, with 18% biaxial strain, the TF model shows $S_{AFM}$ increasing with the system size (with $m_{AFM}$ extrapolating to a non-zero value when $L \to \infty$), indicating an anti-ferromagnetic Mott insulator in the thermodynamic limit. This corresponds to an interac-
tion driven gap of \( \Delta = (0.55 \pm 0.05) \text{ eV} \), comparable to estimates in Ref. [41] obtained by hybrid density functional calculations (Hartree-Fock exchange hybridized with generalized gradient approximation for the exchange-correlation) that do not accurately treat the effects of electron correlations. Moreover, within the Thomas-Fermi method, our QMC calculations find a critical strain of \( \eta_c \approx 0.15 \). Notice that in this case, \( U = U - V = 3.4 t < U_c \) demonstrating that the suggestion by Ref. [19] for mapping the long range Hubbard model for graphene into an effective onsite Hubbard model is quantitatively inaccurate.

Although the TF method has no adjustable parameters, it assumes that the Coulomb interaction between \( p_z \) electrons on the same atom and between neighboring atoms is screened in the same way [26]. This assumption slightly overestimates the ratio \( U/V \) giving a smaller critical strain \( \eta_c \) for the SM-AFM transition. On the other hand, the canonical cRPA method ignores bandwidth and low-energy spectral weight reduction originated from integrating out the high-energy bands [32]. This gives rise to artificially weak partially screened Coulomb interactions, resulting in an overestimation of the critical strain \( \eta_c \). Due to finite sizes, the PPP model overestimates the value of \( U \) and \( V \), and the Ohno interpolation underestimates their difference. However, looking at the three models together, we therefore conclude that the profile of the Coulomb potential for realistic graphene lies somewhere in between the TF and cRPA estimates. The TF model gives a maximum Mott gap of more than an order of magnitude larger than room temperature, and this value sets the upper bound for experiments.

In summary, using the best available models in the literature to estimate the effective Coulomb interaction between \( p_z \) electrons in graphene, we have employed quantum Monte Carlo simulations to explore graphene’s phase diagram in response to parameters that can be changed experimentally. We have found, surprisingly, that manipulating the short-range part of the effective Coulomb potential (i.e. the non-universal and material specific component) is the crucial factor in determining the phase of graphene. Most importantly, we show that application of experimentally realistic amounts of isotropic strain is a promising route to cross the SM-AFM quantum phase transition and to observe a strongly correlated state in this otherwise weakly interacting material.

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Given the lack of published QC-PPP computations for strained aromatic hydrocarbon molecules, we have obtained the long range Hubbard model parameters for graphene subject to 18% biaxial strain (i.e. $\eta = 0.18$) from the unstrained $V(r)$ computed by Ref. [33] but with $r \rightarrow (1 + \eta) r$, while the hoping parameter $t$ was obtained from the results of Pereira and co-workers: $t \rightarrow t_0 e^{-3.37\eta}$ (see Ref. [30] for details).