Short-range Coulomb correlations render massive Dirac fermions massless

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Abstract – Tight-binding electrons on a honeycomb lattice are described by an effective Dirac theory at low energies. Lowering symmetry by an alternate ionic potential ($\Delta$) generates a single-particle gap in the spectrum. We employ the dynamical mean-field theory (DMFT) technique to study the effect of on-site electron correlation ($U$) on massive Dirac fermions. For a fixed mass parameter $\Delta$, we find that beyond a critical value $U_{c1}(\Delta)$ massive Dirac fermions become massless. Further increasing $U$ beyond $U_{c2}(\Delta)$, there will be another phase transition to the Mott insulating state. Therefore, the competition between the single-particle gap parameter, $\Delta$, and the Hubbard $U$ restores the semi-metallic nature of the parent Hamiltonian. The width of the intermediate semi-metallic regime shrinks by increasing the ionic potential. However, at small values of $\Delta$, there is a wide interval of $U$ values for which the system remains semi-metal. The implication of this result for graphene is that in contrast to a single-particle picture, the on-site Coulomb repulsion makes the Dirac cone spectrum robust against small values of the symmetry breaking parameter $\Delta$.

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Introduction. – The single-particle spectrum of excitations in graphene [1] can be very accurately described by a tight-binding model involving hopping between the localized $p_z$ orbitals of neighboring carbon atoms [2]. The low-energy sector of such Hamiltonian will be described by a $(2+1)$-dimensional Dirac theory [3]. Starting from this point, many perturbations can be imagined and/or fabricated to modify the spectrum of Dirac electrons [4,5]. From the applications point of view, it is important to open up a gap in the spectrum by lowering the symmetry of the nearest-neighbor tight-binding Hamiltonian. For example, the substrate can induce a sub-lattice symmetry breaking, e.g., by adding an alternate ionic potential of strength $\Delta$, which immediately leads to a charge gap of magnitude $2\Delta$ in the spectrum of single-particle excitations and renders the Dirac electrons massive [6,7], the ground state of which will be a trivial band insulator (BI). Recent \textit{ab initio} estimates of the strength of the Hubbard $U$ in graphene suggests that the on-site Coulomb repulsion is quite remarkable, $\sim10$ eV [8]. Since this value is expected to be a local property of $p_z$ orbitals in carbon atoms, one does not expect the above value of $U$ to be much different when the Dirac fermions of the underlying honeycomb lattice acquire a mass due to extrinsic effects, such as substrate, binding with ad-atoms such as hydrogen [9], etc. Therefore, it is important to consider the competition between the single-particle gap parameter $\Delta$ and the Hubbard parameter $U$ on top of a semi-metallic state at half-filling. On the strongly correlated limit, when the Hubbard energy scale dominates over the ionic potential, \textit{i.e.}, $U \gg \Delta$, the system will be a Mott insulator (MI) where the charge fluctuations become costly because of the no-double-occupancy constraint imposed by large $U$, while in the opposite limit where $\Delta$ dominates over $U$, the system can be described in terms of an effective massive Dirac theory. The purpose of this paper is to show that short-range many-body Coulomb interaction $U$ can transform massive Dirac fermions into massless ones.

The threefold coordination of carbon atoms on the honeycomb lattice of graphene is the basic mathematical reason for the emergence of cone-like dispersion in graphene which is responsible for semi-metallic properties. If the dimension and/or coordination number were different, the parent one-band tight-binding Hamiltonian would, at half-filling, describe a metal. A previous DMFT study by Garg and coworkers predicts that for metallic...
parent Hamiltonians, the intermediate phase will be a metal [10], i.e., the competition between Hubbard and ionic terms in a metal, restores the metallic state. One may ask the same question for semi-metallic (Dirac) systems: What would be the result of competition between the Hubbard and ionic terms in a semi-metal? Would the intermediate phase be a metal? Or will the competition between the Hubbard and ionic terms—both of which would individually drive the system towards insulating behavior—give way to the semi-metallic behavior?

To tackle this question, the dynamical mean-field theory (DMFT) is a suitable and powerful method [11], which is capable of handling Hubbard interaction in a proper way. This approximate technique becomes exact in the limit of infinite coordination numbers [11,12] which can be formally incorporated by the assumption of a higher-dimensional generalization of various lattices [11,13]. For lower coordination number, the local (k-independent) self-energy employed in the DMFT becomes only an approximate description. Hence, the most significant drawback of the method is expected to be the underestimation of the spatial quantum fluctuations [14–16]. Therefore, the values of the critical parameters obtained from a simple DMFT on the honeycomb geometry may be overestimated [17]. However, the overall picture emerging from this numerically powerful method is expected to hold even when more sophisticated alternative techniques, such as cluster DMFT [18], Gutzwiller projection [19], quantum Monte Carlo [20] or slave-particle [21] schemes, are employed. Since in this work we are not interested in fine spectral details, the lack of k-resolution we believe will not affect the central conclusion of the paper, namely that the semi-metallic behavior is restored when Hubbard term and ionic potential compete.

The ionic-Hubbard model has been studied extensively in one dimension [22], and two dimensions, and the nature of the intermediate phase has been debated [23]. In addition to various low-dimensional techniques employed to study such model, the DMFT technique has also been employed to study the nature of the intermediate phase of this model for metallic parent systems [10,24]. In ref. [10] the authors implemented DMFT for the Bethe lattice and found that by increasing U for fixed Δ, the system undergoes two phase transitions: First from band insulator into metallic phase, and second from metal into Mott insulator phase [10]. However in ref. [24] they used almost the same method and find the coexistence insulator phase region for some Δ, U [24].

Model and method. – The ionic-Hubbard Hamiltonian on the honeycomb lattice with two atoms in same unit cell is given by

\[
H = -t \sum_{i \in A, j \in B} [c_{i \sigma}^\dagger c_{j \sigma} + \text{h.c.}] + \Delta \sum_{i \in A} n_i - \Delta \sum_{i \in B} n_i + U \sum_i n_{i \uparrow} n_{i \downarrow} - \mu \sum_i n_i,
\]

where \(t\) is the nearest-neighbor hopping, \(\Delta\) denotes the ionic potential which alternates sign between the site in sub-lattice \(A\) or \(B\). The Hubbard \(U\) stands for the repulsion potential between two electrons with opposite spins in the \(i\)-th site of the lattice. The chemical potential is \(\mu = U/2\) at half-filling and so the average filling factor is \(\langle n_A \rangle = \langle n_B \rangle = 1\). The model for \(t > 0\) and non-interacting limit \(U = 0\), represents a band insulator, with energy gap \(E_{\text{gap}} = 2\Delta\). The average filling factors at half-filling will become \(\langle n_A \rangle = 0, \langle n_B \rangle = 2\). For \(U \gg \Delta\), the system is in the Mott insulator phase with \(n_A = n_B = 1\) [25]. In the intermediate region, a flow equation analysis shows that at some energy scale, the ionic and Hubbard terms are expected to cancel each other’s effect [25].

To formulate the DMFT machinery for a semi-metallic parent system, consider a parent tight-binding Hamiltonian on the honeycomb lattice in the paramagnetic phase. The interaction Green’s function in the bipartite lattice acquires a matrix form as

\[
G(\vec{k}, \omega) = \begin{pmatrix} \zeta_A(\vec{k}, \omega^+) & -\epsilon(\vec{k}) \\ -\epsilon(\vec{k}) & \zeta_B(\vec{k}, \omega^+) \end{pmatrix},
\]

where \(\vec{k}\) is the momentum vector in the first Brillouin zone, \(\epsilon(\vec{k})\) is the energy dispersion for the honeycomb lattice [2], and \(\zeta_A(\vec{k}) = \omega^+ + \Delta + \mu - \Sigma_A(\omega^+)\) with \(\omega^+ = \omega + i0^+\). In DMFT approximation the self-energy, \(\Sigma_A(\omega^+)\) is local [11], i.e., the self-energy matrix is diagonal and independent of \(\vec{k}\). Therefore, the off-diagonal elements vanish. Hence the local Green’s function corresponding to sub-lattice \(a = A, B\) can be written as \(G_a(\omega^+) = \sum_{\vec{k}} G_{a\vec{k}}(\vec{k}, \omega^+)\), which simplifies to [10]

\[
G_a(\omega^+) = \zeta_a(\omega^+) \int_{-\infty}^{\infty} \frac{\rho_0(\epsilon)}{\zeta_a(\omega^+) \zeta_B(\omega^+) - \epsilon^2} d\epsilon,
\]

where \(a = A(B), \bar{a} = B(A)\) and \(\rho_0(\epsilon)\) is the bare DOS of the honeycomb lattice [2].

We start with an initial guess for the filling factor and self-energy [10]. Then we determine the host Green’s function from Dyson’s equation \(G^{-1}_0(\omega^+) = G^{-1}_a(\omega^+) + \Sigma_a(\omega^+)\). Afterwards, we solve the impurity problem and find \(\Sigma_a(\omega^+) = \zeta_a \langle G_0(\omega^+) \rangle\). In this step we use the iterated perturbation theory (IPT) as impurity solver [11]. The iteration of these steps continues until convergence is reached. After convergence, we calculate the density of states given by \(\rho_0(\omega) = -\frac{1}{\pi} \text{Im} \text{Tr}[G_0(\vec{k}, \omega^+)/\pi]\). The particle-hole symmetry at half-filling leads to \(\rho_A(\omega) = \rho_B(-\omega)\), for the DOS of the two sub-lattices. The total
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DOS for the honeycomb lattice is eventually obtained via
\[ \rho(\omega) = \rho_A(\omega) + \rho_B(\omega). \]

**Results and discussion.** In fig. 1, we have shown the converged results for three typical values of \( U \) at a constant \( \Delta = 0.1t \). As can be seen in this overall picture which covers the whole range of energies in the bandwidth, for small values of \( U \), we have a simple band gap in the spectrum which has single-particle character. As \( U \) increases, the spectral weight is transferred to higher energies to form upper and lower Hubbard bands. The striking feature in fig. 1 is that, despite the formation of Hubbard bands at larger values of \( U \), the overall shape of the low-energy spectral features resembles that of the parent Hamiltonian. The DOS around the Fermi level is V shaped at energy scales above \( \sim \Delta \), and the van-Hove singularity arising due to the saddle point in the band structure moves towards lower energies.

In fig. 2 we have zoomed in the lowest-energy scales around the Fermi level. As can be clearly seen in this figure, increasing \( U \) eventually closes the single-particle gap, and restores the linear DOS at all low-energy scales, including those below \( \sim \Delta \), and renders the system semi-metallic. To our knowledge, *this is a rare instant where many-body interactions of relativistic fermions effectively removes their mass and makes them massless.* By further increasing \( U \), up to \( 11t \), the spectral transfer to upper and lower Hubbard bands becomes higher and higher (fig. 1), while at the same time a Mott-Hubbard gap appears around the Fermi surface as in fig. 2. Therefore, at a fixed value of \( \Delta \), as one increases \( U \), there will be a phase transition at \( U_{c1} \) to the parent semi-metallic phase, followed by another phase transition at larger \( U_{c2} \) to the Mott insulating phase. The intermediate phase is characterized by a strictly linear DOS in the low-energy scales, which qualifies the intermediate phase for an effective Dirac theory. Note that the Fermi velocity in the intermediate effective \( 2+1 \) Dirac theory is renormalized with respect to the effective Dirac theory of the parent Hamiltonian. In fig. 3, we show converged results for three typical \( U \) values in the intermediate regime which indicate the decrease in the Fermi velocity of the intermediate Dirac liquid phase as a function of \( U \) which ultimately leads to a SMIT [14].

Repeating such calculations for a range of ionic potentials \( \Delta \), we map out the phase diagram for the ionic Hubbard model on the honeycomb lattice, the boundaries of which are represented by blue and red lines in fig. 4. First of all for \( \Delta \approx 0 \), the width of the band insulating (BI) phase diminishes which is equivalent to \( U_{c1} \approx 0 \), and there will be only one phase transition separating SM and MI phases [14–16]. Note that the vertical axis denotes values of \( U/W \), where \( W \) is the bandwidth of the parent Hamiltonian. As can be seen in fig. 4, by increasing \( \Delta \), the SM region becomes narrower, and beyond \( \Delta/t \sim 0.5 \— the energy scale up to which the Dirac cone linearization
holds—the red and blue boundaries merge. Beyond this point, the phase transition will be essentially between the BI and MI phases.

For comparison in fig. 4 we have also reproduced the data from ref. [10] for a metallic parent Hamiltonian with Bethe lattice DOS. One interesting difference between the intermediate region on the honeycomb and Bethe lattice is that in the former case, the ground state of the parent Hamiltonian (SM) occupies a much larger region in the two-dimensional space of \( \frac{\Delta}{t} \) and \( \frac{U}{W} \). This could be interpreted as the robustness of the parent phase of the Dirac electrons compared to Schroedinger electrons when an ionic and Hubbard energy scales compete. One more conclusion that could be drawn from fig. 4 is that if we imagine a horizontal line at a constant \( U/W \sim 0.5-0.7 \) which may be relevant to graphene [8], it can be seen that for a range of \( \Delta/t \sim 0.04-0.05 \), the system still remains in the SM phase. For a reasonable estimate of \( t \sim 2.7-3 \) eV, this implies that graphene can remain SM even in the presence of a symmetry breaking ionic potential of strength \( \Delta \sim 110-150 \) meV. Such a single-site DMFT may have overestimated the upper boundary \( U_{c2}(\Delta) \) [17]. Improving on these calculations by, e.g., cluster extension of DMFT is expected to push the upper boundary down, and hence our estimate of the tolerance \( \Delta \sim 110-150 \) meV is not expected to change much.

Normally the gap magnitudes in gapped graphene samples are assumed to satisfy \( E_{\text{gap}}^{(0)} = 2\Delta \). However, this picture holds when one completely ignores the many-body effects. Hence we have used the superscript “0” to emphasize that it is the “non-interacting” gap. In fig. 5 we plot the actual spectral gap as a function of \( U \) for a fixed value of \( \Delta = 0.1t \). As can be seen the actual (interacting) gap strongly depends on the interaction parameter \( U \) in both band and Mott insulating phases. In particular, the value of the gap corresponding to \( U \sim 4t \) which is relevant to graphene, at \( \Delta = 0.1t \sim 280 \) meV is expected to be less than half of the non-interacting estimate. Hence without proper account of the on-site correlations [8], the estimates of \( \Delta \) based on the observation of \( E_{\text{gap}} \) is expected to be about a factor of two underestimated.

### Summary and discussions

We studied the ionic-Hubbard model on honeycomb lattice by the DMFT method, and we found the system undergoes two phase transitions by increasing \( U \) for \( \Delta > 0 \). For \( U < U_{c1}(\Delta) \) the system is in the band insulator phase whose effective low-energy theory is the \( (2+1) \)D massive Dirac theory. For the \( U_{c1}(\Delta) < U < U_{c2}(\Delta) \) region the competition between \( U \) and \( \Delta \) energy scales restores the semi-metallic character of the parent Hamiltonian and makes them massless Dirac fermions. This is in agreement with the renormalization group analysis presented in ref. [4], where a symmetry broken charge density wave (CDW) state enters a semi-metallic phase before entering the strong-coupling antiferromagnetic (AF) phase when the Hubbard \( U \) increases. However, it should be noted that the origin of the spectral gap in the \( U = 0 \) limit of ref. [4] is the longer-range Coulomb interaction which opens a CDW gap, while in our case, \( \Delta \) has been entered phenomenologically as a symmetry breaking field whose precise nature can be quite arbitrary. Ultimately, for \( U > U_{c2}(\Delta) \) the strong correlations transform the intermediate SM to a Mott insulator [14]. Beyond \( \Delta \sim 0.5t \), the upper and lower critical lines approach each other and the semi-metallic region will be so narrow that it will disappear. This theoretical study has implications for gapped graphene samples. The observed values of the spectral gap is always below the “non-interacting” value of \( 2\Delta \). An implication of this result for Dirac fermions, e.g., in graphene is that due to a substantial value of \( U \), the very small value of...
Short-range Coulomb correlations render massive Dirac fermions massless symmetry breaking $\Delta$ cannot open a single-particle gap in the spectrum. This can be interpreted as robustness of the Dirac cone spectrum against symmetry breaking interactions, which is due to on-site Coulomb repulsion. The strong renormalization of the gap magnitude is not the only manifestation of the Hubbard correlations $U$. It also strongly influences other spectral features such as the lifetime of quasi-particles, e.g., in hydrogenated graphene [26].

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