Dynamical Mean Field Study of The Dirac Liquid

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Renormalization is one of the basic notions of condensed matter physics. Based on the concept of renormalization, the Landau’s Fermi liquid theory has been able to explain, why despite the presence of Coulomb interactions, the free electron theory works so well for simple metals with extended Fermi surface (FS). The recent synthesis of graphene has provided the condensed matter physicists with a low energy laboratory of Dirac fermions where instead of a FS, one has two Fermi points. Many exciting phenomena in graphene can be successfully interpreted in terms of free Dirac electrons. In this paper, employing dynamical mean field theory (DMFT), we show that an interacting Dirac sea is essentially an effective free Dirac theory. This observation suggests the notion of Dirac liquid as a fixed point of interacting 2+1 dimensional Dirac fermions. We find one more fixed point at strong interactions describing a Mott insulating state, and address the nature of semi-metal to insulator (SMIT) transition in this system.

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INTRODUCTION

Dirac theory of electrons was formulated in 1928 to describe the relativistic motion of electron waves [1]. This theory not only is consistent with the spin \( \hbar/2 \) of electron, but also obeys the correct relativistic covariance. Now days, accelerators and neutron stars are not the only places to search for Dirac fermions. Advances in science and technology has enabled physicists to realize Dirac fermions in energy scales as low as 1 eV, or even lower in solid state physics. The nodal quasiparticles of d-wave cuprate superconductors being one example in superconducting state of matter [2].

Recently, graphene, a single atomic layer of graphite, was fabricated [3], which has initiated a rapidly growing research activity in condensed matter physics [4]. The low-energy electronic structure of this system is approximately described by a 2+1 dimensional Dirac theory [5], which enjoys a chiral symmetry [5, 6]. Therefore graphene, the unrolled carbon nanotube; provides the condensed matter with a laboratory for the relativistic fermions on the table top [7].

There is still another road to search for Dirac fermions in material physics laboratory. Recent advances in ultra cooling and atom trap methods [8] have elevated this technology to a chip based level [9]. This provides a unique opportunity for tuning the interaction parameters in microscopic models employing the so called Feshbach resonance [10]. These motivate the study of strongly interacting fermions on honeycomb lattice in parameters regimes, much beyond what can be currently realized in graphene, or high \( T_c \) cuprates.

The three-fold coordination for hopping of fermions on a honeycomb lattice is responsible for the relativistic low-energy theory [5], which strictly speaking describes a semi-metallic state of a Dirac sea; rather than a metallic state of a Fermi sea. This semi-metal is described by a pseudo-gap in the density of states (DOS) shown in Fig. 1. Such feature in DOS is also relevant to the nodal quasi particles of high \( T_c \) cuprate superconductors [2].

While the single particle Dirac theory seems to work well in graphene, it is important to search for interesting many-body effects on honeycomb lattice. For example the possibility of \( f \)-wave or \( d + id \)-wave superconductivity [11, 12, 13, 14], as well as CDW instability [11] on honeycomb lattice has been discussed. Perturbative renormalization group studies [15] has indicated that the long range part of the Coulomb interaction is irrelevant, and gives rises to a non interacting fixed point. In this paper we focus on the short range part of the interaction, employing a non-perturbative method of DMFT. This theory has been very successful in addressing the question of metal to insulator transitions [17]. According to the prediction of DMFT, the onset of transition to Mott insulating phase is accompanied by formation of the so called Kondo resonance, the spectral weight of which characterizes the quasi-
particle weight \( Z \) of the underlying Fermi sea. In the case of a half-filled Dirac sea, instead of an extended Fermi surface, one has to deal with two Fermi points at the so called \( K \) points of the Brillouin zone. Due to the cone like dispersion of the conduction and valence band near these points, there will be no quasi particle state at the Fermi level \([4]\). Hence the quasi-particle weight \( Z \) of Fermi liquids can not be used to discuss the transition to Mott insulating regime.

In this work we employ the DMFT approximation to study the SMIT of Dirac liquids in two dimensional honeycomb lattice. The picture which emerges from this study is that; for weak to moderate interaction strengths, the Dirac sea state remains stable against local many body interactions. The sole role of interactions would be to renormalize the Dirac quasi particles. Such robustness of the Dirac fermions against many body interactions has been observed in various measurements in graphene \([18]\). For strong enough interactions, a Mott insulating state is stabilized. We study some simpler model density of states which mimic the true 2D DOS of graphene Eq. 4. We find the value of \( U_c \sim 13.3 t \), which is not sensitive to the details of DOS.

**MODEL AND METHOD**

We take the tight-binding electrons on honeycomb lattice \([4]\), which give rise to Dirac spectrum near the \( K \) points of the Brillouin Zone (BZ), and add a short ranged Coulomb interaction of Hubbard type to it:

\[
H = -t \sum_{\langle i,j \rangle} c_{i \sigma}^\dagger c_{j \sigma} + \text{h.c.} + U \sum_{j} \left( n_{j \uparrow} - \frac{1}{2} \right) \left( n_{j \downarrow} - \frac{1}{2} \right)
\]  
(1)

where the hoping amplitude for \( p_z \) electrons in graphene is \( t \sim 2.7 eV \), while for the atoms trapped in optical lattices it is typically on the scale of \( t \sim \mu K \sim 10^{-10} eV \). Through the paper when the units are not specified, the units in which \( t = \hbar = 1 \) is implied. Also we take the atomic separation to be 1. This model is manifestly particle-hole symmetric and the Hartree term at half filling (\( \langle n_{j \sigma} \rangle = 1/2 \)) vanishes.

In the absence of interaction, the Hamiltonian becomes

\[
H_0 = \begin{pmatrix} 0 & -f(k) \\ -f^*(k) & 0 \end{pmatrix}
\]  
(2)

where \( k = (k_x, k_y) \), and \( f(k) = \epsilon^{ik \cdot d_1} + \epsilon^{ik \cdot d_2} + \epsilon^{ik \cdot d_3} \) (Fig. 1). The eigenvalues of this matrix are \( \varepsilon_k = |f(k)|. \) When the above complex function \( f(k) \) linearized around the Fermi points \( K, K' \) of the BZ, gives rise to the Hamiltonian \( H = \pm v_F \sigma \cdot k \). The DOS for this non interacting system is given by \([19]\).

\[
\rho(\varepsilon) = \frac{1}{\sqrt{z_0}} F\left( \frac{\pi}{2} \sqrt{\frac{Z_1}{z_0}} \right),
\]  
(3)

where

\[
Z_0 = \begin{cases} 
(1 + |\varepsilon|)^2 - (\varepsilon^2 - 1)^2/4; & |\varepsilon| < 1 \\
4|\varepsilon|; & 1 \leq |\varepsilon| \leq 3 \end{cases}
\]  
(4)

and

\[
Z_1 = \begin{cases} 
4|\varepsilon|; & |\varepsilon| < 1 \\
(1 + |\varepsilon|)^2 - (\varepsilon^2 - 1)^2/4; & 1 \leq |\varepsilon| \leq 3 \end{cases}
\]  
(5)

Here \( F(\pi/2, x) \) is the complete elliptic integral of first kind \([20]\). At low energies where the dispersion becomes \( \varepsilon_k = \pm v_F k \), we have linear energy dependence in the pseudo-gap shaped DOS (Fig. 2).

\[
\rho(\varepsilon) = 2\pi v_F^{-2} |\varepsilon|
\]  
(6)

where \( h v_F = 3ta/2 \) is the bare Fermi velocity of quasiparticles at the Fermi points. In Fig. 2 we have plotted the DOS for two and infinite dimensional (hyper)honeycomb lattice \([21]\).

In DMFT, one starts with a local free propagator \( g_{0\alpha}(\omega) \), where the Greek indices \( \alpha, \beta \) etc. correspond to sub-lattices A,B. Next and most important part of the DMFT consists in employing an impurity solver to obtain the local self-energy \( \Sigma_\alpha \) as a functional of \( g_{0\alpha} \). Note that, within the single-site DMFT approximation the self-energy is purely local \([17]\) which means the off-diagonal self-energies vanish and it can be described by the diagonal matrix elements \( \Sigma_{\alpha}(\omega) \). We use the iterated perturbation theory to solve the impurity problem:

\[
\Sigma_\alpha(t) = U^2 g_{0\alpha}(t) g_{0\alpha}(t^-).
\]  
(7)

Now using this self-energy we construct the Green’s function of the honeycomb lattice which can be written as

\[
G_{\alpha\beta}(k, \omega) = \left( \frac{\zeta_A(k, \omega) - f(k)}{-f^*(k)} \zeta_B(k, \omega) \right)^{-1},
\]  
(8)

where \( k \) belong to the first BZ of sub-lattice, and \( \zeta_\alpha(k, \omega) = \omega - \varepsilon_k + \mu - \Sigma_\alpha(\omega) \). The half filled band which
gives rise to a Dirac sea, due to the bipartite nature of the honeycomb lattice corresponds to $\mu = 0$. Such half-filling condition corresponds to undoped graphene, whereas in optical lattices with one species atom, it corresponds to half atom per site. Note that the particle-hole symmetry can also be used which implies $\Sigma_A(\omega) = -\Sigma_B(-\omega)$. To connect the lattice Green’s function to local one, we need to project onto sub-lattice $A(B)$, which reads

$$g_\alpha(\omega) = \xi_\alpha \sum_k \frac{1}{\xi_A \xi_B - \varepsilon_k^2} = \xi_\alpha \int d\varepsilon \frac{\rho(\varepsilon)}{\xi_A \xi_B - \varepsilon^2}$$

where $\rho(\varepsilon)$ is the DOS of massless Dirac fermions, Eq. (3). To close the set of equations, we only need to append the Dyson equation

$$g_\alpha^{-1}(\omega) = g_0^{-1}(\omega) - \Sigma_\alpha(\omega)$$

We solve the set of equations (7), (8), (9) and (10) self-consistently.

**RESULTS**

The Hilbert transformation in equation (9) is the only place where the band structure (DOS) of system enters the DMFT machinery. Using the DOS of realistic graphene given in Eq. (3) we obtain the interacting DOS for various values of $U < U_c \approx 13.3t$ shown in Fig. 3. As can be seen, upon increasing $U$, the spectral weight is transferred to higher energies, accompanied by a increase in the slope of the DOS. Interpreting the results in terms of Eq. (6) one sees that (i) the Dirac nature of the spectrum is preserved, manifested in the linear DOS and the pseudo-gap structure around the charge neutrality point is preserved for all $U < U_c$, but with a reduced Fermi velocity $v_F$ replacing the non-interacting Fermi velocity $v_F = 3/2$. (ii) As there are no quasiparticle states at the Fermi level for the Dirac fermions, the SMIT is not accompanied by a Kondo resonance at the Fermi surface. (iii) The (logarithmic) van Hove singularity of the band structure corresponding to saddle point at the M point of the Brillouin zone persists.

For the DOS Fig. 3 the Hilbert transformation must be done with a numerical quadrature with typically $N_a = 2000$ abscissas for a Simpson quadrature to achieve the double precision accuracy needed in typical self-consistency problems. We simplify the DOS of graphene with a parameter dependent prediction formula (9) we obtain figure 4. Panels (a), (b) correspond to $h = 0$ and (c), (d) denote $h = 1$. We see that this model DOS produces the essential features (i)-(iii) above. For small to intermediate values of $U$ one can see the renormalization of the slope in (a), (c). Comparison of (a), (c) shows that this feature is qualitatively independent of the presence or lack of a singularity. Singularity places initially at $|\varepsilon| = \pm 1$ moves to lower energies as one increases $U$. Panels (b), (d) show the SMIT for $h = 0, h = 1$, respectively. For $h = 0$, we obtain $U_{hc}^{h=0} \approx 13.3t$, while for $h = 1$, the critical value is slightly lower. Right at the critical point, due to critical slowing down, it is extremely difficult to obtain convergence. The
The model DOS corresponding to $\tilde{\text{v}}_F$ interpolates to zero at the quantum critical point (QCP) $U_c \approx 13.3t$. Unlike the MIT in metallic systems with extended Fermi surface, there is no Kondo resonance corresponding to quasiparticle at the Fermi level. Therefore SMIT can not be described in terms of the spectral weight $Z$ of such resonant state. Instead the $\tilde{\text{v}}_F$ in Fig. 5 can be identified as an order parameter characterizing a Dirac liquid state. Beyond a QCP at $U_c \approx 13.3t$, a Mott insulating state appears.

The semi-metal to insulator transition in $D = \infty$ honeycomb lattice (Dotted line in Fig. 2) has been previously studied by Santoro and coworkers [21], where they focused on the zero and finite temperature magnetic phase transitions. They find that at zero temperature, at a critical value of $U_c^\infty \approx 2.3W$ there is a phase transition from a paramagnetic semi-metal to an anti-ferromagnetic Mott insulator, where $W$ is the band width. If one takes this as a ad hoc critical value for $D = 2$ honeycomb lattice with $W = 6t$, one expects a critical value of $U_c^\infty \approx 13.8t$ in 2D honeycomb lattice, which is very close to the value $13.3t$ we find here. Sorella and Tosatti approached the same problem by quantum Monte Carlo methods [22]. They found a zero temperature SMIT between a non magnetic semi-metal and an anti-ferromagnetic insulator at a critical value of $U_c^{\text{QMC}} \approx 4.5t$. The Brinkman-Rice analysis of the SMIT within the Gutzwiller approximation gives a critical value of $U_c^{\text{BR}} \approx 12.8t$ [23], which is again rather close to the value we obtain. The corresponding mean field value is $U_c^{\text{MF}} \approx 2.23t$. Such a significant difference between the mean field and more accurate methods indicates the importance of quantum fluctuations in SMIT.

FIG. 5: (Color online) Renormalization of the Dirac fermions velocity $\tilde{\text{v}}_F$ by the Hubbard $U$ term.

In this paper we studied the zero temperature phase transition of Dirac fermions on a honeycomb lattice. Our results can be applied to atoms in honeycomb optical lattices, as well as electrons in undoped graphene. We studied the nature of SMIT in this system. We found no quasiparticle resonance state. The renormalized Fermi velocity $\tilde{\text{v}}_F$ was suggested as an order parameter for a Dirac liquid separated from a Mott insulator by a QCP at $U_c \approx 13.3t$. The recent renormalization in $\tilde{\text{v}}_F$ seen in ARPES measurements [18] can not be solely described in terms of electron-phonon or electron-plasmon interactions of a doped graphene. Such renormalization arising from Hubbard term may also contribute to those seen in ARPES measurements.

Others have also reported on a quantum critical point behavior of Dirac fermions using large $N$ expansion, beyond which an insulating phase emerges [24]. The renormalization group flow equations for quartic perturbations [25] indicate possible insulating phase at strong couplings. Foster and Aleiner find logarithmic divergences using large $N$ renormalization group approach [16]. They found that the long range part of the Coulomb interaction enhances the short range part of the interaction. Our method addresses the role of short range part in a non-perturbative DMFT sense, which therefore can be regarded as a complementary analysis to their’s.

Gonzalez and coworkers find within renormalization scheme that the Coulomb interactions drive the system to a non-interacting fixed point [15]. Their finding agrees with the Dirac Liquid fixed point in our analysis. However our non-perturbative DMFT analysis indicates another Mott insulating fixed point in addition to the Dirac liquid fixed point of Ref. [15] in agreement with our exact and non-perturbative analysis.

In graphene samples $U \approx 6$ eV, which is not strongly correlated, places them at $U/t \sim 2.2$, far from the Mott insulating phase. However, one can describe the graphene starting from a Mott insulating valence bond (RVB) point. In such a description one needs to allow for charge fluctuations on top of an RVB ground state [13]. This provides an opportunity for high temperature superconductivity in ~ 20% doped graphene [12, 14].

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