Electron-electron interactions and Dirac liquid behavior in graphene bilayers


Department of Physics, Boston University, 590 Commonwealth Ave., Boston, MA 02215

We study the effect of electron-electron interactions in the quasiparticle dispersion of a graphene bilayer within the Hartree-Fock-Thomas-Fermi theory. We find that the electronic fluid can be described in terms of an effective Lorentz invariant theory with renormalized mass and velocity, the Dirac liquid. We show that the Dirac liquid can quantitatively describe recent cyclotron resonance experiments in this system.

PACS numbers: 81.05.Uw,51.35.+a,71.10.-w

Since graphene was isolated in 2004 [1], it has attracted attention because of its possible application in all-carbon based electronic devices [2] and its connections to relativistic field theory [3]. While there is strong theoretical [4] and experimental evidence [2,5] that single layer graphene (SLG) behaves as essentially a weakly interacting gas of two-dimensional (2D) Dirac particles, the situation in bilayer graphene (BLG) is much less clear. Early theoretical studies have indicated that the SLG is much less prone towards magnetic states [6], while BLG can become magnetic at low densities [7]. Moreover, while the electronic compressibility of SLG has essentially features of an insulator [8,9], the BLG compressibility is, unlike the 2D electron gas (2DEG) [10], non-monotonic and strongly dependent on electronic density [11]. It has also been argued that, unlike SLG, BLG should be unstable towards many-body states such as a pseudospin magnet [12], a Wigner crystal [13], and an excitonic superfluid [14]. It has been demonstrated that BLG is a tunable gap semiconductor by application of a transverse electric field [15,16], leading to extra flexibility in dealing with its electronic properties [17,18]. While electrons in BLG have a different topological (Berry’s) phase than electrons in SLG, as evident in integer quantum Hall effect measurements [19], the experimental evidence for electron-electron interaction effects in BLG has been elusive. Nevertheless, recent cyclotron resonance experiments in bilayer graphene [20] have shown departures from the non-interacting bilayer model proposed by McCann and Falko [21]. These disagreements do not seem to be describable in terms of disorder effects alone [22]. The objective of our paper is to clarify these discrepancies and in the process to establish that the graphene bilayer is a Dirac liquid.

The SLG has a honeycomb lattice structure that leads to a Dirac-like electronic dispersion, $E(k) = \pm v_F |k|$, at the edges (the K and K’ points) of the Brillouin zone. The electrons are described in terms of a 2D “relativistic” Dirac Hamiltonian with zero rest mass, where the velocity of light, $c$, is replaced by the Fermi-Dirac velocity, $v_F$. In the BLG (Bernal structure) the two graphene layers are rotated by a relative angle of $\pi/3$ that breaks the sublattice symmetry leading to 2 pairs of massive Dirac particles at the K (K’) point. Nevertheless, the system remains metallic because 2 bands, belonging to different pairs, touch in a point. More explicitly, the non-interacting bands have the form:

$$E_1(k) = -mv_F^2 + E(k), \quad E_2(k) = mv_F^2 - E(k),$$

$$E_3(k) = mv_F^2 + E(k) \quad \text{and} \quad E_4(k) = -mv_F^2 - E(k),$$

where $E(k) = \sqrt{(mv_F^2)^2 + (v_F k)^2}$. Hence, $E_1(k)$ and $E_4(k)$ ($E_2(k)$ and $E_3(k)$) describe a massive relativistic dispersion with rest mass energy given by $mv_F^2$. Rotations by other angles do not break the sublattice symmetry and hence do not lead to mass generation [22].

In this paper we establish that BLG behaves as a Dirac liquid, namely, a liquid of Dirac quasiparticles with renormalized mass and velocity. The situation described here is unique when compared to standard non-relativistic Fermi liquids such as $^3\text{He}$ [24] and ordinary metals [25], or even to relativistic Fermi liquids such as quark matter in the core of neutron stars [26]. On the one hand, while the electrons in graphene are effectively “relativistic”, in the sense that they obey an effective Lorentz invariance (only true at low energies) with the Dirac velocity playing the role of velocity of light, on the other hand, from the point of view of an external observer, the whole graphene system is Galilean invariant and non-relativistic since the Dirac velocity is much smaller than the actual speed of light. As a consequence, electron-electron interactions, just as in the case of relativistic [26] and non-relativistic [24] Fermi liquids, renormalize the quasiparticle mass, but unlike the relativistic and non-relativistic Fermi liquids, the “velocity of light” is also renormalized.

The Coulomb interaction between electrons breaks the effective Lorentz invariance of the non-interacting problem since it can be thought as instantaneous from the point of view of the electrons. In BLG, this violation of Lorentz invariance leads to the famous upward logarithmic renormalization of the Fermi-Dirac velocity originally proposed in Ref. [27]. That effect is a result of the lack of screening in the SLG due to the vanishing of the density of states. The BLG, however, has a finite density of states at the Dirac point and hence screening plays an important role [28]. We show that, similarly to the 2DEG [25], the Hartree-Fock (HF) theory alone leads to an unphysical logarithmic singularity at the Fermi surface indicat-
ing the importance of screening in this system. When screening is accounted through the Thomas-Fermi theory, the log singularity is suppressed and, surprisingly, full Lorentz invariance is recovered. We show that this result is due to the suppression of the intra-band transitions relative to the inter-band transitions. In renormalization group sense, the fixed point that describes the problem is effectively Lorentz invariant with a renormalized effective mass, $m^*$, and renormalized Fermi-Dirac velocity, $v_F^*$, which are dependent on the interaction (in analogy to the dependence of the effective mass with Landau parameters in a Fermi liquid \[24\]). This unexpected result indicates that BLG can be described in terms of a Lorentz invariant Dirac liquid. In order to test our findings, we study the problem of cyclotron resonance in this system and find good quantitative agreement with recent measurements \[20\].

We use a tight binding description of BLG in which only the in-plane, $t \approx 3\text{eV}$, and the out-of-plane, $t_\perp \approx 0.37\text{eV}$, nearest hopping parameters are considered \[30\]. In this case we have $v_F = 3t_a/2 \approx 1.42\text{Å}$ and $mv_F^2 = t_{\perp}/2$. From now on we choose units such that $\hbar = 1 = v_F$. The hyperbolic shape of the non-interacting dispersion introduces an intrinsic energy scale in the problem, $\lambda$. In the “non-relativistic” (NR) limit, $k \ll m$, one can replace the four hyperbolic bands by two parabolic bands $E_{\pm}(k) = \pm k^2/2m$ \[21\]. In this approximation, the usual NR dispersion of the 2DEG is recovered, but with allowed negative energy values. In the “ultra-relativistic” (UR) limit, $k \gg m$, $E(k) \sim k$, one obtains the SLG dispersion. The crossover energy scale from non-relativistic to ultra-relativistic (NR-UR) is given by $m$. We notice that the effective non-relativistic low energy approximation fails when treating the interacting problem because the Coulomb energy associated with electron-electron interactions is of the order of the inter-band transitions \[11\].

The electronic interactions are included by adding to the non-interacting energy $E_0 = 1/\pi^2 \sum_i \int E_i(p)\,dp$ an exchange term which can be written as (energies are given per unit area, and the spin and valley degeneracy factor of 4 is accounted):

$$E_{ex} = -\sum_{i,j=\alpha} \int \chi^\alpha_{ij}(\mathbf{q}, \mathbf{p})\chi^\alpha_{ji}(\mathbf{p}, \mathbf{q}) n_i(\mathbf{q}) n_j(\mathbf{p}) V_\alpha(\mathbf{q} - \mathbf{p}) \quad (1)$$

where $\alpha = \pm 1$ correspond to the symmetric/antisymmetric representations of the Coulomb interaction:

$$V_\pm(\mathbf{k}) = 2\pi e^2/\epsilon(1 \pm \exp(-kd))/(2(k + \beta m)), \quad (2)$$

$n_i(\mathbf{q})$ is the occupation number of band $i$, and $\chi^\alpha_{ij}(\mathbf{q}, \mathbf{p})$ are overlap matrices which contain information of the change of basis \[2\]. Screening is taken into account through the Thomas-Fermi approximation by introducing a screening length in \[2\] that is proportional to the density of states, that is, to the effective mass. In \[2\] $\beta$ is the parameter that controls the value of the Thomas-Fermi screening length \[2\], the HF theory is obtained by taking $\beta = 0$. The energy of a quasiparticle in the $i^{th}$ band is given by $\epsilon_i(\mathbf{q}) = \delta E/\delta n_i(\mathbf{q})|_{n_i = n_i^0}$, where $\delta n_i(\mathbf{q}) = n_i(\mathbf{q}) - n_i^0(\mathbf{q})$, being $n_i^0(\mathbf{k})$ the occupation number of the non-interacting system. $E[\delta n_i]$ is the total energy $E = E_0 + E_{ex}$. We can therefore write $\epsilon_i(\mathbf{q}) = E_i(\mathbf{q}) + \Delta E_i(\mathbf{q})$ with:

$$\Delta E_i(\mathbf{q}) = -4 \int \sum_{\alpha, j} \chi^\alpha_{ij}(\mathbf{q}, \mathbf{p}) \chi^\alpha_{ji}(\mathbf{p}, \mathbf{q}) n_j^0(\mathbf{p}) V_\alpha(\mathbf{q} - \mathbf{p}), \quad (3)$$

the correction to the non-interacting band $E_i(\mathbf{q})$.

We consider the case of electron doping such as that the chemical potential does not reach the uppermost band, which is usually the experimentally realized situation \[31\]. Therefore, our results are valid for Fermi energies up to $\sqrt{2}t_{\perp}$, which corresponds to densities smaller than $n_e \approx 10^{13} \text{ cm}^{-2}$. We look then...
The divergence in the quasiparticle velocity disappears for finite $\beta$. The most striking feature of our calculations is that the quasiparticle dispersion can be fitted by

$$\epsilon_1(k) = \epsilon_0 + \sqrt{(v_F^* k)^2 + (m^* v_F^*)^2},$$

(4)

where $\epsilon_0$ is a constant, and $m^*$ and $v_F^*$ are the quasiparticle mass and renormalized “light” velocity, respectively. We find that this result is valid to high accuracy for a large region of energy and momenta due to the fact that the inter-band transitions largely dominate over the intra-band ones.

The results for $m^*/m$ and $v_F^*/v_F$ are shown in Fig. 3 as a function of electronic density, $n_c = k_F^2/\pi$, for different values of the screening strength $\beta$. Note that $v_F^*/v_F$ increases monotonically with density, whereas $m^*/m$ has a minimum at a finite $n_c$. While $m^*/m$ is renormalized to smaller values, $v_F^*/v_F$ is renormalized to larger values. This has interesting consequences for the NR-UR crossover mentioned earlier. The crossover energy for the non-interacting problem is given by $E_c = m v_F^2$. Analogously, for the interacting result we can define the crossover energy as $E_c^* = m^* (v_F^*)^2$. This quantity is plotted in Fig. 4 (b), which shows that $E_c^* > E_c$ for all the values of the parameters (this is also true if we vary the coupling constant $0.1 \leq g \leq 2$). However, the relevant parameter to compare with experiment is the crossover electronic density, $n_c = q_c^2/\pi = (m v_F^2)^2/\pi$, that is, the density at which the NR-UR crossover takes place. Fig. 4 (a) shows the renormalized value of this quantity, $n_c^* = (m^* v_F^*)^2/\pi$, in units of the non-interacting value $n_c$. Indeed, it is seen that $n_c^* < n_c$ always, even though the renormalized quasiparticles’ energy is higher.

Let us now consider the problem in the presence of a transverse magnetic field $B$. For the non-interacting problem, the Landau levels are given by (restoring units [33])

$$
\frac{E_{\pm}}{\omega_c} = \pm \left\{ n + \frac{1}{2} + 2r^2 - \frac{1}{2} \left[ 1 + 16r^4 + 16r^2 \left( n + \frac{1}{2} \right)^2 \right]^{1/2} \right\}^{1/2}
$$

(5)
where $n$ is a positive integer, $\omega_c = \sqrt{2eB/cv_F}$ is the cyclotron frequency, and $r = mv_F^2/\omega_c$. One can clearly see that this problem has the NR-UR crossover as a function of $B$ discussed earlier. At low fields, $r \gg 1$, we find $E^+_n \approx \pm (\omega_c^2/(2mv_F^2)) \sqrt{n(n+1)}$, and the Landau level energy is proportional to $B$ as in the NR problem [21]; at high fields, $r \ll 1$, one finds $E^+_n \approx \pm \omega_c \sqrt{n}$ and, as in the UR case, we find the Landau level energy proportional to $\sqrt{B}$.

Just as in the case of a Fermi liquid, in the Dirac liquid the quasiparticles carry electric charge $e$ and couple to a magnetic field via minimal coupling ($p \to p - ieA/c$ where $A$ is the vector potential such that $B = \nabla \times A$). Hence, the Landau level spectrum is the same as the non-interacting problem, eq. (5), with the bare parameters, $m$ and $v_F$, replaced by renormalized ones, $m^*$ and $v_F^*$, respectively. In Fig. 5 we show the data from cyclotron resonance experiments [20] for inter-Landau level transitions for different filling factors $\nu = n_e/n_{Fb}$ ($n_{Fb}$ is the density of flux quanta through the system) together with our results for $g = 0.5$, $\beta = 1$ such that $v_F^* \approx 10^6$ m/s and $t_{\perp}^* = 2m^*(v_F^*)^2 \approx t_{\perp}/3 \approx 0.12$ eV ($v_F \approx 0.5 \times 10^6$ m/s and $t_{\perp} \approx 0.37$ eV). The values of $v_F^*$ and $m^*$, as shown above, depend on the electronic density so they have a slightly different value for each $\nu$, this was taken into account for the plots in Fig. 5. One can see that our results are in quantitative agreement with the experimental data, giving support to the idea that this system is indeed described by a Dirac liquid of quasiparticles described by a dispersion given by (4). Note however that we are not attempting a self-consistent calculation in which the screening would also depend on the density.

We have studied the effect of electron-electron interactions on the electronic properties of a graphene bilayer within the Hatree-Fock-Thomas-Fermi theory. We have shown that due to the dominance of inter-band transitions in the electronic dispersion, the quasiparticles can be effectively described by a Dirac liquid of quasiparticles with internal Lorentz invariance but renormalized velocity and rest mass. This state of affairs is unlike what happens in non-relativistic and relativistic Fermi liquids, putting bilayer graphene in a different class of quantum fluids. Furthermore, we have tested our calculations by comparing our results with recent cyclotron resonance experiments and found quantitative agreement between theory and experiment.

The authors wish to thank A.H. MacDonald, Johan Nilsson and A. K. Geim for their valuable comments on the manuscript.

[29] If we follow the analogy with the 2DEG, $\beta = 4g$.
[30] Other hopping parameters are smaller in magnitude [32] and usually suppressed by disorder [22].