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Electron-electron interactions in graphene bilayers

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Abstract – We study the effect of electron-electron interactions in the quasiparticle dispersion of a graphene bilayer within the Hartree-Fock-Thomas-Fermi theory by using a four-bands model. We find that the electronic fluid can be described by a non-interacting-like dispersion but with renormalized parameters. We compare our results with recent cyclotron resonance experiments in this system.

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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 [5,8,9], 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 Fal'ko [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.

The SLG has a honeycomb lattice structure that leads to a Dirac-like electronic dispersion, $E(\mathbf{k}) = \pm\tilde{c}|\mathbf{k}|$, 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, \tilde{c} . 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: $E_1(\mathbf{k}) = -m\tilde{c}^2 + E(\mathbf{k})$, $E_2(\mathbf{k}) = m\tilde{c}^2 - E(\mathbf{k})$, $E_3(\mathbf{k}) = m\tilde{c}^2 + E(\mathbf{k})$ and $E_4(\mathbf{k}) = -m\tilde{c}^2 - E(\mathbf{k})$, where $E(\mathbf{k}) = \sqrt{(m\tilde{c}^2)^2 + (\tilde{c}\mathbf{k})^2}$. Hence, $E_1(\mathbf{k})$ and $E_4(\mathbf{k})$ ($E_2(\mathbf{k})$ and $E_3(\mathbf{k})$) describe a massive relativistic dispersion with rest mass energy given by $m\tilde{c}^2$. Rotations by other angles do not break the sublattice symmetry and hence do not lead to mass generation [23].

Our results suggest that BLG behaves as 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 ^3He [24] and ordinary metals [25], or even to relativistic Fermi liquids such as quark matter in the core of neutron stars [26]. 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 renormalized¹. Moreover, in BLG as well as in SLG the existence of negative-energy bands and a pseudo-spin degree of freedom has to be included when constructing a Fermi liquid theory. This has been analyzed microscopically in refs. [27,28] and through a phenomenological model in ref. [29] for SLG, however, a treatment of BLG which takes into account its full hyperbolic four-bands structure is missing.

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 SLG, this violation of Lorentz invariance leads to the famous upward logarithmic renormalization of the Fermi-Dirac velocity originally proposed in ref. [30]. 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 [31]. We show that, similarly to the 2DEG [25], the Hartree-Fock (HF) theory alone leads to an unphysical logarithmic singularity at the Fermi surface indicating the importance of screening in this system. When screening is accounted through the Thomas-Fermi (TF) theory, the log singularity is suppressed and, surprisingly, 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 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, $t \approx 3$ eV, and the out-of-plane, $t_{\perp} \approx 0.37$ eV, nearest-neighbor hopping parameters are considered². In this case we have $\tilde{c} = 3ta/2$ ($a = 1.42$ Å) and $m\tilde{c}^2 = t_{\perp}/2$. From now on we choose units such that $\hbar = 1 = \tilde{c}$. The hyperbolic shape of the non-interacting dispersion introduces an intrinsic energy scale in the problem, m . 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

¹Note that the mass renormalization in both the non-relativistic and relativistic Fermi liquid is directly associated to the Galilean or Lorentz invariance of the system, see refs. [24,26].

²Other hopping parameters are smaller in magnitude [32] and usually suppressed by disorder [22].

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 $E_0 = 1/\pi^2 \sum_i \int E_i(p) d\mathbf{p}$ 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):

$$E_{ex} = -2 \sum_{i,j,\alpha} \int_{p,q} \chi_{ij}^{\alpha}(\mathbf{q}, \mathbf{p}) \chi_{ji}^{\alpha}(\mathbf{p}, \mathbf{q}) n_i(q) n_j(p) V_{\alpha}(\mathbf{q} - \mathbf{p}), \quad (1)$$

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

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

$n_i(q)$ is the occupation number of band i , and $\chi_{ij}^{\alpha}(\mathbf{q}, \mathbf{p})$ are overlap matrices which contain information of the change of basis [7]. Screening is taken into account through the TF approximation by introducing a screening length in (2) that is proportional to the density of states. In (2) β is the parameter that controls the value of the TF screening length; the HF theory is obtained by taking $\beta = 0$. Within the Random Phase Approximation (RPA), $\beta_{RPA} = 4g(1 + E_F/m)$, being $g = e^2/\hbar\tilde{c}$ the dimensionless coupling constant, and E_F the Fermi energy. For experimentally realized densities ($n_e \approx 10^{11} - 10^{13} \text{ cm}^{-2}$) and $g = 0.5$ ($\epsilon = 3.9$ for SiO_2), $\beta \approx 1 - 5$. The energy of a quasiparticle in the i -th band is given by $\epsilon_i(q) = \delta E / \delta n_i(\mathbf{q})|_{n_i = n_i^0}$, 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 $\epsilon_i(q) = E_i(q) + \Delta E_i(q)$ with $\Delta E_i(q) = -4 \int_q \sum_{\alpha,j} \chi_{ij}^{\alpha}(\mathbf{q}, \mathbf{p}) \chi_{ji}^{\alpha}(\mathbf{p}, \mathbf{q}) n_j^0(p) V_{\alpha}(\mathbf{q} - \mathbf{p})$ the correction to the non-interacting band $E_i(q)$.

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 situation³. 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 at the correction to the first band, which we write as $\Delta E_1(q) = D_+(q, k_F) + D_-(q, \Lambda)$ to distinguish intra-band (D_+) from inter-band (D_-) contributions. The expressions for D_{\pm} can be easily derived from $\Delta E_1(q)$. k_F is the Fermi wave vector and Λ a cutoff of the order of the inverse lattice spacing ($\Lambda \approx 1 \text{ \AA}^{-1} \approx 7 \text{ eV}$).

Figure 1 shows the quasiparticle band within the HF theory (solid line) for a typical value of the Fermi vector. Figure 1(a) depicts the correction due to the intra-band transitions, D_+ . Its behavior, as expected, is qualitatively very similar to that of a 2DEG [25]. In particular, the inflection point seen at $q \approx k_F$ is due to the special role of k_F which separates a domain with an avoidable

³The case of hole doping is analogous, except for a small asymmetric term [11] which we discuss later.

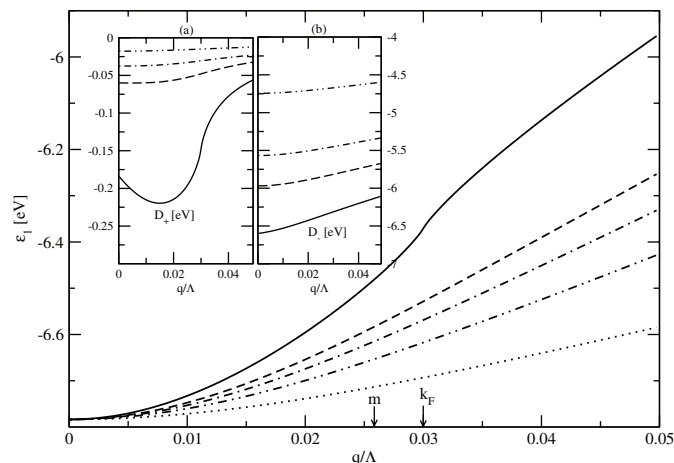


Fig. 1: Quasiparticle dispersion, $\epsilon_1(q)$ (in eV), as a function of the momentum q (in units of Λ). Inset: intra- (D_+) and inter- (D_-) band contributions. Full line: $\beta = 0$ (HF); dashed line: $\beta = 1$; dash-dotted line: $\beta = 2$; dash-double-dotted line: $\beta = 5$; dotted line: non-interacting value. Curves have been shifted for comparison ($k_F/\Lambda = 0.03$ and $g = 0.5$).

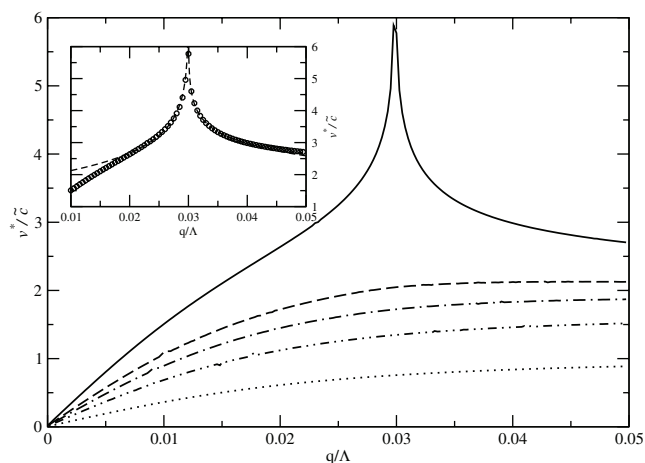


Fig. 2: $v^*(q)$ (in units of \tilde{c}) as a function of q (in units of the cutoff Λ) for $k_F/\Lambda = 0.03$. Dotted line: non-interacting value. Solid line: HF. Dashed line: TF with $\beta = 1$; dash-dotted line: $\beta = 2$; dash-double-dotted line: $\beta = 5$. Inset: zoom-in near the Fermi vector and the logarithmic fit to the divergence (dashed line) for HF.

singularity $q \leq k_F$ from a singularity free domain for $q > k_F$. While D_+ diminishes with k_F , the correction due to D_- is independent of it. The latter is shown in fig. 1(b). As can be seen from the figure, for typical electronic densities, the correction due to inter-band interactions is roughly two orders of magnitude bigger than that of the intra-band. Notice, from fig. 1, that the quasiparticle dispersion, however, inherits the inflection point from D_+ at $q = k_F$. The renormalized band velocity is given by $v^*(q) = |\partial\epsilon/\partial q|$, which is plotted in fig. 2. Due to the sharp inflection point in ΔE_1 at k_F , the effective quasiparticle

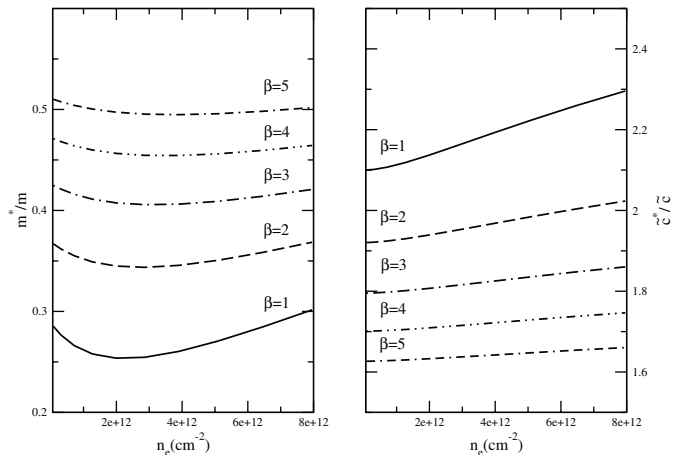


Fig. 3: Left: m^* (in units of the bare mass m) as a function of the electron density n_e (in units of electrons per cm^{-2}). Right: \tilde{c}^* (in units of the bare velocity \tilde{c}) as a function of n_e , for different β ($g = 0.5$).

Fermi velocity, $v^*(k_F)$, presents an unphysical logarithmic divergence: $v^*(k \sim k_F) \sim -4g/\pi \log(|k - k_F|/\Lambda)$, as it occurs for the 2DEG. For small momentum nevertheless, $q/k_F \ll 1$, the renormalized dispersion can be shown to be parabolic: $\epsilon_1(q) \approx q^2/(2\tilde{m})$, with $\tilde{m}^{-1} = m^{-1} + g(5/k_F - 1)/2$.

As mentioned earlier, the divergence of the Fermi velocity is an unpleasant feature of the HF approximation which indicates the necessity of introducing screening in the problem. The renormalized band $\epsilon_1(q)$ is shown in fig. 1 for different values of β . We see that the introduction of screening eliminates the inflection point at k_F . This can be seen clearly in fig. 2, where it is shown that the divergence in the quasiparticle velocity disappears for finite β . The most striking feature of our calculations is that the quasiparticle dispersion can be fitted by a non-interacting-like dispersion:

$$\epsilon_1(k) = \epsilon_0 + \sqrt{(v_F^* k)^2 + (m^* \tilde{c}^*)^2}, \quad (3)$$

where ϵ_0 is a constant, and m^* and \tilde{c}^* 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 ones⁴.

The results for m^*/m and \tilde{c}^*/\tilde{c} are shown in fig. 3 as a function of the electronic density, $n_e = k_F^2/\pi$, for different values of the screening strength β . Note that, for fixed β , \tilde{c}^*/\tilde{c} increases monotonically with density, whereas m^*/m has a minimum at a finite n_e . While m^*/m is renormalized to smaller values, \tilde{c}^*/\tilde{c} is renormalized to larger values. This has interesting consequences for the NR-UR crossover mentioned earlier. The crossover energy

⁴Note that the quasiparticle Fermi velocity, $v^*(k_F)$ is not inversely proportional to the effective mass (as in the usual Fermi liquid case), but to the quasiparticle energy.

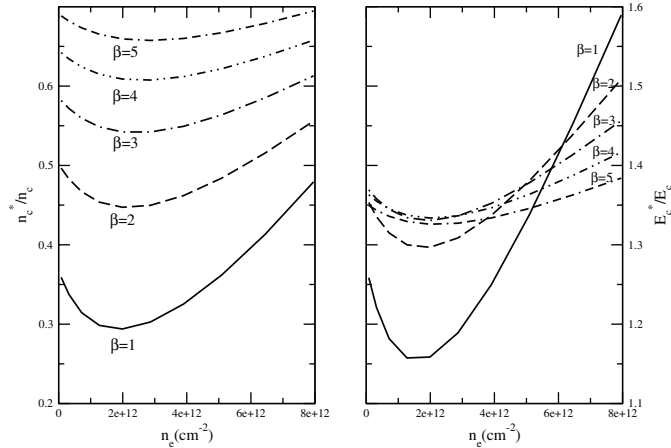


Fig. 4: Left: NR-UR crossover density n_c^* (in units of the bare crossover density n_c) as a function of electronic density n_e (in units of electrons per cm^{-2}). Right: E_c^* (in units of the non-interacting crossover energy E_c) as a function of n_e , for different β ($g = 0.5$).

for the non-interacting problem is given by $E_c = m\tilde{c}^2$. Analogously, for the interacting result we can define the crossover energy as $E_c^* = m^*(\tilde{c}^*)^2$. 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, $n_c = q_c^2/\pi = (m\tilde{c})^2/\pi$, that is, the density at which the NR-UR crossover takes place. Figure 4(a) shows the renormalized value of this quantity, $n_c^* = (m^*\tilde{c}^*)^2/\pi$, 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]:

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

where n is a positive integer, $\omega_c = \tilde{c}\sqrt{2eB}/c$ 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 $E_n^\pm \approx \pm[\omega_c^2/(2m\tilde{c}^2)]\sqrt{n(n+1)}$, and the Landau level energy is proportional to B as in the NR problem [21]; at high fields, $r \ll 1$, one finds $E_n^\pm \approx \pm\omega_c\sqrt{n}$ 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, here the quasiparticles carry electric charge e and couple to a magnetic field via minimal coupling. Note that here, however, the cyclotron mass is not protected by Kohn's theorem

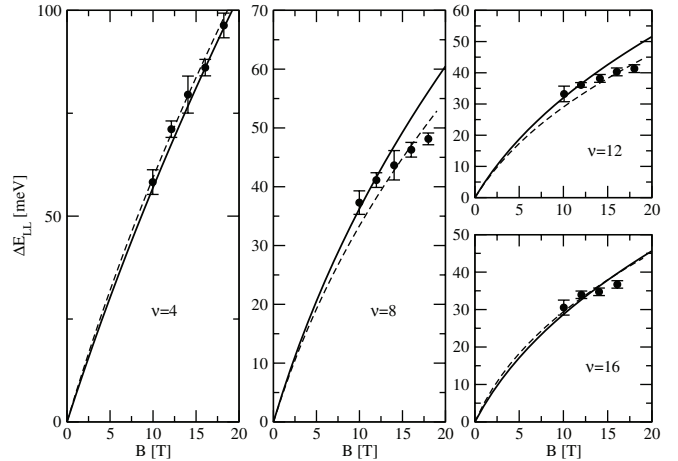


Fig. 5: Landau level transition energies for different filling factors $\nu = 4$ ($n: 0 \rightarrow 1$), $\nu = 8$ ($n: 1 \rightarrow 2$), $\nu = 12$ ($n: 2 \rightarrow 3$) and $\nu = 12$ ($n: 2 \rightarrow 3$) as a function of B (in tesla). The experimental data (dots) was taken from ref. [20]. The solid line is the theoretical value for $g = 0.5$, and $\beta = 4$ for bare values $\tilde{c} \approx 0.76 \times 10^6$ m/s and $t_\perp \approx 0.33$ eV. The dashed line shows the fits obtained in ref. [20] for $t_\perp = 0.35$ eV.

since the dispersion is not parabolic [34]⁵. Hence, the Landau level spectrum is the same as the non-interacting problem, eq. (4), with the bare parameters, m and \tilde{c} , replaced by renormalized ones, m^* and \tilde{c}^* , respectively. In fig. 5 we show the data from cyclotron resonance experiments [20] for inter-Landau level transitions for different filling factors $\nu = n_e/n_\Phi$ (n_Φ is the density of flux quanta through the system) together with our results for $g = 0.5$, $\beta = 4$, $\tilde{c} = 0.76 \times 10^6$ m/s ($\tilde{c}^* = 1.2 - 1.3 \times 10^6$ m/s) and $t_\perp \approx 0.33$ eV ($t_\perp^* = 0.44 - 0.45$ eV). These values were obtained by fitting our renormalized theory to the experimental data, taking β , g , and the bare m and \tilde{c} as free parameters, and are in agreement with recent infrared spectroscopy data [35]. The variation of \tilde{c}^* and m^* with the electronic density was taken into account, however, we took the screening strength β as fixed, since our treatment is not self-consistent. Nevertheless, as a double check, the value obtained for g is the expected for BLG on SiO_2 and β falls within the expected range for such densities. One can see that our results are in fair quantitative agreement with the experimental data, giving support to the idea that this system can be described by a Dirac liquid of quasiparticles with a dispersion given by (3). There is a small electron-hole asymmetry due to inter-band interactions (and therefore independent of density), which results in smaller values of t_\perp^* ($\sim 10\%$) and \tilde{c}^* ($\sim 5\%$) for hole doping. This difference, however, is not enough to explain the asymmetry observed in [20]. As was mentioned above,

⁵Kohn's theorem might be expected to be asymptotically valid in the NR limit. However, given the renormalization of the UR-NR crossover to lower electronic densities, this would be the case only at very low densities. In the dilute limit inhomogeneities [5], Wigner crystallization [11,13] and ultimately the trigonal warping term [21] would also be relevant.

the screening strength β was fitted to a constant value for all four plots in fig. 5, and it should be taken as the best average β that gives a reasonable good fit for all the data range. For a better agreement with the data it would be probably necessary to include self-consistently the dependence of β with the electronic density but this goes beyond the scope of the present paper.

We have studied the effect of electron-electron interactions on the electronic properties of a graphene bilayer within the Hartree-Fock-Thomas-Fermi theory by taking into account the full four-bands model of BLG. We have shown that the quasiparticles can be described by a non-interacting, Lorentz-like dispersion with renormalized parameters which depend on the electronic density. The fact that the Lorentz invariance of the dispersion is recovered for a large range of energies is an unexpected result since there is no evident symmetry behind it. It is important to note that this result is due to the dominance of inter-band transitions, which are missing in the usual Fermi liquid picture. Since this contribution is independent of electronic density, the accuracy of the effective description increases with decreasing density. Further investigation is needed to determine if corrections beyond HF lead to deviations from the Lorentz dispersion. Furthermore, we have tested our calculations by comparing our results with recent cyclotron resonance experiments and found quantitative agreement between theory and experiment. Our results are also in agreement with recent *ab initio* calculations [36].

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