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Charge density excitations in bilayer graphene in high magnetic field

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The charge-density excitations in bilayer graphene at the filling-factor $\nu \ll 1$ at small momenta are considered in the frame of the Hartree-Fock approximation. The presence of small asymmetry of graphene layers is included. The dependence of the magnetoplasmon energy on the bilayer ground state is shown. The energy splitting proportional to $\sqrt{H}$ for the symmetric case with half-filled zero-energy levels is found both for bilayer and monolayer graphene.

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Recent experimental progress has allowed the fabrication and study of monolayer and bilayer graphene. The electronic band structure of these objects is gapless and has a chirality [1]. The monolayer has Dirac-type spectrum with linear dispersion and chirality exhibiting Berry phase π. In magnetic field there is zero-energy Landay level, fourfold degenerate due to two spins and two valleys. The bilayer graphene is the unique object which combines the parabolic dispersion law of quasiparticles with their chirality exhibiting Berry phase 2π. In magnetic field there is a double-degenerate zero-energy Landay level incorporating two different orbital states with the same energy. Taking into account spin and valley degeneracies, the zero-energy Landau level is eightfold degenerate. For the bilayer with small asymmetry there are four weakly split two-fold levels, close to zero. This one-electron structure was confirmed in experiments on integer quantized Hall effect and Shubnikov-de Haas oscillations [2, 3]. These properties are understood in terms of non-interacting electrons. The electron-electron interaction is an important problem in the study of cyclotron resonance in monolayer [4, 5], bilayer [6] and multilayer [7, 8] graphene. There are experiments with multilayer graphene exhibiting some properties of a monolayer structure, using magnetotransmission measurements [9 - 11]. The charge-density excitations at small momenta are considered in the frame of the Hartree-Fock approximation for monolayer graphene [12, 13]. In [14, 15] electromagnetic response in graphene was considered theoretically in RPA approximation. In [16] intra-Landau level transitions are considered.

In this work inter-Landau-level transitions from the top filled to the next free Landau levels in the bilayer graphene have been studied. Charge density excitations (magnetoplasmons) are considered. These types are more useful for experimental study (it is possible to observe their energy by inelastic light scattering or microwave absorption). The charge-density excitations at small momenta are considered in the frame of the Hartree-Fock approximation. The case of filling-factor $\nu \ll 1$ is considered. This filling-factor means the absence of free carriers due to doping or applied voltage. The presence of small asymmetry is included. The energy of magnetoplasmon excitations is considered and the dependence of the magnetoplasmon energy on the bilayer ground state is shown. It is shown that the energy splitting proportional to $\sqrt{H}$ for the symmetric case with half-filled zero-energy levels takes place for bilayer and monolayer graphene.

The bilayer is modelled as two coupled hexagonal lattices with inequivalent sites (A1, B1) and (A2, B2) in the first and second graphene layers, respectively, arranged according to Bernal (A2-B1) stacking. The asymmetry between on-site energies in the two layers Δ is taken into account. The low-energy states of electrons in (A1-B2) dimer are conveniently described by an effective two-component Hamiltonian [17] that operates in the space of wave functions $\Psi = (\psi_{A1}, \psi_{B2})$ in the valley K and of $\Psi = (\psi_{B2}, \psi_{A1})$ in the valley $\tilde{K}$.

$$H = -\frac{1}{2m}\begin{pmatrix} 0 & (\pi^+)^2 \\ \pi^2 & 0 \end{pmatrix} + \frac{\xi\Delta}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{\xi\Delta v^2}{\gamma_1^2}\begin{pmatrix} \pi^+\pi & 0 \\ 0 & -\pi\pi^+ \end{pmatrix}, \quad (1)$$

where $\pi = p_x + p_y$, $\xi = 1$ in valley K, $\xi = -1$ in $\tilde{K}$, $m = \gamma_1/2v^2$, $v = \frac{\sqrt{3}}{2\hbar}a\gamma_0$.

Coupling parameters $\gamma_1 = \gamma_{A_2B_1}$, $\gamma_0 = \gamma_{A_1B_1} = \gamma_{A_2B_2}$, a is the lattice constant.

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Without magnetic field, the parameter of asymmetry Δ gives rise to the gap in the spectrum $\sim \Delta$. The two-component Hamiltonian is applicable within the energy range of $|\varepsilon| < \frac{1}{4}\gamma_1$, for magnetic fields $H < c\gamma_1/2ve$. For $\gamma_1 = 0.39$ meV it corresponds to $H < 50$ T.

The Landau level spectrum is found using the Landau gauge $\mathbf{A} = (0, Bx)$, π^+ and π are raising and lowering operators in the basis of functions $\phi_{Nk} = e^{iky}\phi_N(x-k)$ [18]. At small asymmetry the resulting spectrum contains two states with energies close to zero

$$E_{0\xi} = \frac{1}{2}\xi\Delta, \quad E_{1\xi} = \frac{1}{2}\xi\Delta - \xi\delta, \quad \delta = \Delta\hbar\omega_c/\gamma_1 \quad (2)$$

and for $N \geq 2$ energy levels

$$E_{\pm N\xi} = \pm\hbar\omega_c\sqrt{N(N-1)} - \frac{1}{2}\xi\delta, \quad N \geq 2, \quad (3)$$

which are weakly split in valleys and almost equidistant for $|N| \gg 1$. In the presence of the magnetic field the asymmetry splits the eightfold degenerate zero-energy Landau level into four twofold levels, if the Zeeman splitting is omitted.

We believe that the small asymmetry is important only for filling of LLs and the wave functions may be used without asymmetry.

$$\Psi_{n,k} = a_n\phi_{|n|k} + b_n\phi_{|n|-2,k} \quad (4)$$

$$\Psi_{0k} = (\phi_{0k}, 0), \quad \Psi_{1k} = (\phi_{1k}, 0),$$

$$\Psi_{\pm Nk} = \frac{1}{\sqrt{2}}(\phi_{Nk}, \pm\phi_{N-2,k}). \quad (5)$$

Note that the spectrum of high-energy LLs is applicable in such fields that $\hbar\lambda_H < \gamma_1/2v$. For higher fields the full four-band Hamiltonian has to be used to determine the exact LL spectrum [19, 20]. Trigonal warping is not included, magnetic field is sufficiently high for that. According to [18] $B > B_c, B_c \sim 1$ T. Although in graphite the electron g-factor is not small ($g = 2$), a very light effective mass $m \approx 0.054$ in the bilayer determines a small ratio between the Zeeman energy and LL splitting $\varepsilon_Z/\hbar\omega_c \sim 0.05$ [18].

The total Hamiltonian of the many-body system with the Coulomb interaction is

$$\hat{H} = \sum E_{n\xi}a^+_\lambda a_\lambda + H_{\rm int}, \quad (6)$$

where a^+_λ and a_λ are the one-particle creation and annihilation operators; $\lambda = (n, k, \xi, \sigma)$; $n = 0, 1, \pm N$; ξ and σ are valley and spin indexes; k is the parameter which labels degenerate states within one Landau level in Landau gauge. The Coulomb interaction conserves spin and valley indexes.

$$H_{int} = \frac{1}{2}\sum V'(q)\tilde{J}_{n_4,n_1}(q)\tilde{J}_{n_3,n_2}(-q)a^+_{\lambda 1}a^+_{\lambda 2}a_{\lambda_3}a_{\lambda 4}, \quad (7)$$

$$V'(q) = V(q)e^{iq_x(k_1-k_2-q_y)}, \quad V(q) = \frac{2\pi}{\varepsilon q}, \quad (8)$$

$$\tilde{J}_{m,n}(q) = a^*_n a_m J_{|m||n|}(\mathbf{q}) + b^*_n b_m J_{|m|-2,|n|-2}(\mathbf{q}); \quad (9)$$

$$J_{m,n}(\mathbf{q}) = \left(\frac{n!}{m!}\right)^{1/2} e^{-\frac{q^2}{4}}\left(\frac{q_y + iq_x}{\sqrt{2}}\right)^{m-n} L_n^{m-n}\left(\frac{q^2}{2}\right), \quad (10)$$

$$J_{m,n}(\mathbf{q}) = J^*_{n,m}(-\mathbf{q}), \quad m > n.$$

Magnetic field is high: $E_c \ll \omega_c$, where $E_c = e^2/\varepsilon l_H$, l_H is the magnetic length. Corresponding operators for excitations with momentum K are

$$Q^+_{\lambda\lambda'}(K) = \sum_k a^+_{\lambda'}a_\lambda. \quad (11)$$

The problem is considered in the way analogous to that employed in [12, 13] for monolayer graphene systems. The time-dependent Hartree-Fock approximation is used. The Hartree-Fock approach assumes that E_c is smaller than one-electron transition energy. For monolayer graphene the ratio $E_{10}/E_c = 2.77$ [12] and it is not dependent on the value of the magnetic field. For bilayer graphene $E_c = 10\sqrt{B}$, $\hbar\omega_c = 2.2\,\mathrm{H}$ [17] and the ratio $\hbar\omega_c/E_c = 0.22\,\mathrm{H}^{1/2}$ under the assumption $\epsilon = 5$. For the first nonzero transition $E_{12} = \sqrt{2}\omega_c$, and therefore for $H = 40$ T the ratio $E_{12}/E_c \simeq 2$. We consider the charge-density excitations: valley and spin indexes (ξ, σ) are not changed, $\lambda' = ((n', k+K, \xi, \sigma)$, $\lambda = (n, k, \xi, \sigma)$.

$$E_{n,n';\xi,\sigma} = E_{n'\xi} - E_{n\xi} + E^c_{n,n';\xi,\sigma}. \quad (12)$$

The excitation energy consists of noninteracting and Coulomb parts. Coulomb part E_c is represented by direct ("excitonic" E_{ex}), exchange ("depolarization" – RPA), and exchange self-energy Σ_n contributions to the excitation energy. Restriction for $K \simeq 0$ enables to consider excitations with different (ξ, σ) independently (RPA part is zero).

$$Q^+_{\lambda\lambda'}(0) = Q^+_{n,n';\xi,\sigma}, \quad E^c_{n,n';\xi,\sigma} = E^{n,n'}_{ex} + \Sigma_{n'} - \Sigma_n. \quad (13)$$

As for monolayer graphene, there is the problem of divergency of exchange self-energy Σ_n due to summation over all filled LLs. The spectrum of monolayer and bilayer graphene described by the model Hamiltonian in unbounded both from above and below. This fact is physically artificial. In [13] the cut-off value on energy or number of LL vas defined. In [12] the semi-empirical way was used to treat the problem. Parameter of electron-electron interaction is fitted for one type of transition to experimental data. For the bilayer graphene the area of parabolic dispersion is less than needed cut-off value, and to consider the four-band Hamiltonian is too complicated problem. We only indicate some common rules where the Coulomb part can be seen.

The case of filling-factor $\nu = 0$ is considered. This filling-factor means the absence of free carriers (holes ore electrons) without magnetic field. The Fermi level is equal to zero. We consider the interlayer electron transitions from the top filled (fully or partially) to the next free (fully or partially) Landau levels with energies nearly ω_c. There are following possible ground states and corresponding transitions.

A. The bilayer with asymmetry: $\Delta \neq 0$. For valley with $\Delta\xi > 0$ we have the top filled LL with $n = -2$ and transition $(-2, 1)$, and for valley with $\Delta\xi < 0$ we have the top filled 0 and 1 LLs and transition $(1, 2)$. The noninteracting part is the same for both types of transitions

$$\omega_c\sqrt{2} + \frac{1}{2}|\Delta - \delta|. \tag{14}$$

Note that taking into account the electron-hole symmetry of one-particle Hamiltonian leads to the fact that $(-2, 1)$ and $(1, 2)$ transitions are really the same and have the same energy ($(-2, 1)$ in electron representation is $(1, 2)$ in hole representation). Taking into account spin we have four transitions with equal energies. Energy splitting due to asymmetry is absent, only additional shift takes place.

B. Ferromagnetic state (difference in energies of spin components): one spin component σ_1 of LLs 0 and 1 is completely filled and the other σ_2 is completely empty in both valleys. There are four transitions $Q^+_{1,2,\xi,\sigma_1}$ and $Q^+_{-2,1,\xi,\sigma_1}$ with the same energy.

C. Difference in energies of valley components. In [21] it is suggested that there is an intrinsic small asymmetry between valleys which is analogous to the ferromagnetic case.

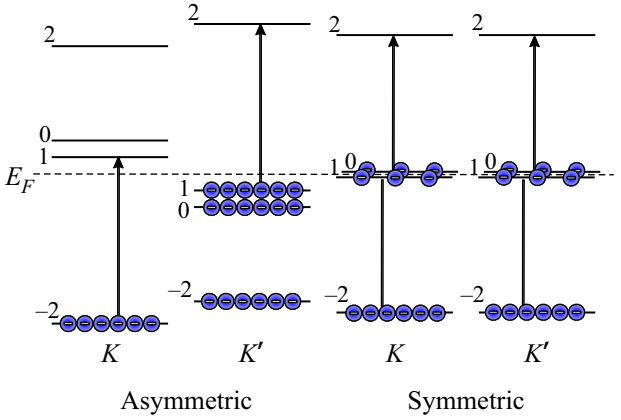
Cases A-C correspond to integer filling.

D. The symmetric ground state with half-filled 0 and 1 LLs in both valleys. For each valley and spin there are two combined $Q^+_{1,2,\xi,\sigma}$ and $Q^+_{-2,1,\xi,\sigma}$ transitions with the same noninteracting part $\omega_c\sqrt{2}$ connected due to Coulomb interaction. It would be possible if the temperature is comparable to Zeeman splitting.

Is bilayer graphene in asymmetric case (A and C) we have filling-factor $\nu = 4$ for the electrons in one valley and $\nu = 4$ for the holes in another valley. In symmetric case we have two half-filled zero-energy levels in both valleys, it means $\nu = 2$ for the electrons in each valley and $\nu = 2$ for the holes in each valley. In all cases we have equal amounts of electrons and holes, it corresponds to $\nu = 0$.

In monolayer graphene with valley asymmetry [12] we have filling-factor $\nu = 2$ for the electrons in one valley and $\nu = 2$ for the holes in another valley. In the valley-symmetric case we have the half-filled zero-energy level in both valleys, it means $\nu = 1$ for the electrons in one valley and $\nu = 1$ for the holes in each valley. In all cases we have equal amounts of electrons and holes, it corresponds to $\nu = 0$.

Therefore, it is necessary to consider the (1,2) electron or hole transitions from filled to the next empty



The energy levels and transitions for symmetric and asymmetric cases

level for A-C cases and combined electron-hole transitions from half-filled to empty levels in the symmetric case (see figure).

For $\nu = 0$ integer filling, labelled $0I$,

$$E^{(1,2)}_{ex,0I} = -\frac{1}{(2\pi)^2}\int d\mathbf{q}V(q)\tilde{J}_{22}(\mathbf{q})\tilde{J}_{1,1}(-\mathbf{q}) =$$

$$= \frac{1}{2(2\pi)^2}\int d\mathbf{q}V(q)(J_{22}(q) + J_{00}(q))J_{11}(q)), \tag{15}$$

$$(\Sigma_2 - \Sigma_1)_{0I} = \int d\mathbf{q}\frac{V(q)}{2(2\pi)^2}(|J_{11}(\mathbf{q})|^2 + |J_{10}(\mathbf{q})|^2 -$$

$$- \int d\mathbf{q}\frac{V(q)}{2(2\pi)^2}(\frac{1}{2}|J_{21}(\mathbf{q})|^2 + \frac{1}{2}|J_{20}(\mathbf{q})|^2) +$$

$$+\int d\mathbf{q}\frac{V(q)}{2(2\pi)^2}\sum_{N=2}|J_{2,N}(\mathbf{q})J^*_{0,N-2}\mathbf{q}|. \qquad (16)$$

This value may depend on solving the divergency problem, but it is not equal to zero. There is no Kohn's theorem [22]. Energy splitting due to asymmetry is absent, only additional shift takes place.

In the symmetric case labelled $0H$ there are half-filled 0 ($\nu_0 = 1/2$) and $1(\nu_1 = 1/2)$ LLs in both valleys. For each valley and spin there are two combined $(1,2)$ – $(-2,1)$ transitions. Using the Hartree-Fock approximation for non-integer filling-factors [23, 24] two combined modes $Q^+_{s,a} = Q^+_{1,2,\xi,\sigma} \pm Q^+_{-2,1,\xi,\sigma}$ are found with energies

$$E_{s,a} = \omega_c\sqrt{2} + E_c^{0H} \pm \frac{1}{2}\tilde{V}. \qquad (17)$$

These modes may be called symmetric and antisymmetric in analogy to modes in semiconductor bilayer.

$$E_c^{0H} = \frac{1}{2}E^{(1,2)}_{ex,0I} + (\Sigma_2 - \Sigma_1)_{0H}, \qquad (18)$$

$$(\Sigma_2 - \Sigma_1)_{0H} \neq \frac{1}{2}(\Sigma_2 - \Sigma_1)_{0I}, \qquad (19)$$

$$\tilde{V} = \frac{1}{(2\pi)^2}\int d\mathbf{q}V(q)\tilde{J}_{12}(\mathbf{q})\tilde{J}_{-2,1}(-\mathbf{q}) =$$

$$= \frac{1}{2(2\pi)^2}\int d\mathbf{q}V(q)|J_{12}|^2(\mathbf{q}) = \frac{1}{2}\sqrt{\frac{\pi}{2}}E_c\cdot\frac{7}{16}, \qquad (20)$$

$\tilde{V} = 2.5\sqrt{H}$ and for $H = 40\,\mathrm{T}$, $\tilde{V} \simeq 15\,\mathrm{meV}$.

This splitting for combined electron-hole transitions from half-filled level is not specific to bilayer graphene. For monolayer graphene with filling-factor $\nu = 0$ for combined $(0,1)$(electron) – $(-1,0)$ (hole) transitions the value of splitting is

$$\tilde{V}_{mg} = \frac{1}{2(2\pi)^2}\int d\mathbf{q}V(q)|J_{01}|^2(\mathbf{q}) = \frac{1}{4}\sqrt{\frac{\pi}{2}}E_c. \qquad (21)$$

This value is practically the same as for bilayer graphene ($\tilde{V}_{mg} \simeq 2.5\sqrt{H}$), but for monolayer graphene it is possible to observe this splitting for lower experimentally used magnetic fields.

Observation of this splitting would be the evidence of Coulomb interaction in graphene. If the splitting could not be clearly resolved, it would still perhaps be possible to detect it experimentally as the line broadening depending on magnetic field as $\sqrt{H}$.

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