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Toward theory of quantum Hall effect in graphene

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We analyze a gap equation for the propagator of Dirac quasiparticles and conclude that in graphene in a magnetic field, the order parameters connected with the quantum Hall ferromagnetism dynamics and those connected with the magnetic catalysis dynamics necessarily coexist (the latter have the form of Dirac masses and correspond to excitonic condensates). This feature of graphene could lead to important consequences, in particular, for the existence of gapless edge states. Solutions of the gap equation corresponding to recently experimentally discovered novel plateaus in graphene in strong magnetic fields are described.

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The properties of graphene, a single atomic layer of graphite [1], have attracted great interest, especially after the experimental discovery [2,3] and (made independently) theoretical prediction [4–6] of an anomalous quantization in the quantum Hall (QH) effect. In this case, the filling factors are $\nu = \pm 4(|n| + 1/2)$, where n is the Landau level index. For each QH state, a four-fold (spin and sublattice-valley) degeneracy takes place. These properties of the QH effect are intimately connected with relativistic like features in the graphene dynamics [7–9].

In recent experiments [10,11], it has been observed that in a strong enough magnetic field, $B \gtrsim 20$ T, the new QH plateaus, $\nu = 0, \pm 1$ and ± 4, occur, that was attributed to the magnetic field induced splitting of the $n = 0$ and $n = \pm 1$ Landau levels (LLs). It is noticeable that while the degeneracy of the lowest LL (LLL), $n = 0$, is completely lifted, only the spin degeneracy of the $n = \pm 1$ LL is removed.

On theoretical side, there are now two leading scenarios for the description of these plateaus. One of them is the QH ferromagnetism (QHF) [12–15] (the dynamics of a Zeeman spin splitting enhancement considered in Ref. 16 is intimately connected with the QHF). The second one is the magnetic catalysis (MC) scenario in which excitonic condensates (Dirac masses) are spontaneously produced [17–20]. For a brief review of these two scenarios, see Ref. 21.

While the QHF scenario is based on the dynamical framework developed for bilayer QH systems [22], the MC scenario is based on the phenomenon of an enhancement of the density of states in a strong magnetic field, which catalyzes electron-hole pairing (leading to excitonic condensates) in relativistic like systems. The essence of this effect is the dimensional reduction $D \to D - 2$ in the electron-hole pairing dynamics and the presence of the LLL with energy $E = 0$ (containing both electron and hole states) in relativistic systems in a magnetic field. This universal phenomenon was revealed in Ref. 23 and was first considered in graphite in Refs. 24, 25.

On technical side, the difference between these two scenarios is in utilizing different order parameters in breaking the spin-sublattice-valley $U(4)$ symmetry of the noninteracting Hamiltonian of graphene. While the QHF order parameters are described by densities of the con-

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served charges connected with diagonal generators of the nonabelian subgroup $SU(4) \subset U(4)$, the order parameters in the MC scenario are Dirac mass like terms. Note that while the latter are bifermion operators which are invariant under 2 + 1 dimensional Lorentz transformations (with the Fermi velocity $v_F \simeq 10^6$ m/s playing the role of light velocity), the QHF charge densities are time like components of the corresponding conserved currents which transform as vectors under the Lorentz transformations.

One may think that the QHF and MC order parameters should compete with each other. However, as will be shown in this paper, the situation is quite different: These two sets of the order parameters *necessarily* coexist, which implies that they have the same dynamical origin. The physics underlying their coexistence is specific for relativistic like dynamics that makes the QH dynamics of the $U(4)$ breakdown in graphene to be quite different from that in bilayer QH systems [22] whose dynamics have no relativistic like features.

Our approach is based on studying the gap equation for the propagator of Dirac quasiparticles. For the description of the dynamics in graphene, we will use the same model as in Refs. 24, 25, in which while quasiparticles are confined to a two-dimensional plane, the electromagnetic (Coulomb) interaction between them is three-dimensional in nature. The dynamics will be treated in the Hartree–Fock (mean field) approximation, which is conventional and appropriate in this case [12,13,17,24,25]. Then, at zero temperature and in the clean limit (no impurities), the gap equation takes the form:

$$G^{-1}(x,y) = S^{-1}(x,y) + i\hbar\gamma^0 G(x,y)\gamma^0 \delta(x_0 - y_0) U_C(\mathbf{x}-\mathbf{y}) - \\ - i\hbar\gamma^0 \mathbf{tr}\,[\gamma^0 G(x,x)]\delta^3(x-y) U_C^{(F)}(0)\,. \qquad (1)$$

Here $x \equiv (x_0, \mathbf{x})$, with $x_0 \equiv t$ being time coordinate, $U_C(\mathbf{x})$ is the Coulomb potential in a magnetic field, given in Eq. (46) in Ref. 25, $U_C^{(F)}(0)$ is its Fourier transform at $\mathbf{k} = 0$, $G^{-1}(x,y)$ is the full inverse quasiparticle propagator, and $S^{-1}(x,y)$ is the bare inverse quasiparticle propagator,

$$iS^{-1}(x,y) = [(i\hbar\partial_t + \mu_0 - \mu_B B\sigma^3)\gamma^0 - v_F \boldsymbol{\pi}\boldsymbol{\gamma}]\delta^3(x-y)\,, \qquad (2)$$

where μ_0 is the electron chemical potential, $\boldsymbol{\pi} = -i\hbar\boldsymbol{\partial} + e\mathbf{A}/c$ is the canonical momentum, and $\mu_B B\gamma^0\sigma^3$ is the Zeeman term (the vector potential $\mathbf{A}$ corresponds to the magnetic field $\mathbf{B}$, $B \equiv |\mathbf{B}|$, μ_B is the Bohr magneton, and the Pauli matrix σ^3 acts on spin indices) [26].

For Dirac matrices $\gamma^0, \boldsymbol{\gamma}$, we use the same representation as in Refs. 17, 25 (xy plane is chosen for graphene). Note that while the second term on the right hand side of Eq. (1) describes exchange interactions, the third one is the Hartree term describing annihilation interactions.

The analysis of gap equation (1) beyond the LLL approximation is a very formidable problem. Because of that, we will utilize the following approximation: the Coulomb potential $U_C(\mathbf{x})$ in the gap equation will be replaced by the contact interaction $G_{\rm int}\delta^2(\mathbf{x})$:

$$G^{-1}(x,y) = S^{-1}(x,y) + i\hbar G_{\rm int}\gamma^0 G(x,x)\gamma^0\delta^3(x-y) - \\ - i\hbar G_{\rm int}\gamma^0 \mathrm{tr}\,[\gamma^0 G(x,x)]\delta^3(x-y)\,, \qquad (3)$$

where $G_{\rm int}$ is a dimensional coupling constant. Such an approximation is common in quantum chromodynamics (QCD), where long range gluon interactions are replaced by contact (Nambu–Jona–Lasinio) ones. This leads to a good description of nonperturbative dynamics in low-energy region in QCD (for a review, see, for example, Ref. 27). Because of the universality of the MC phenomenon and because the symmetric and kinematic structures of the gap equations (1) and (3) are the same, we expect that approximate gap equation (3) should be at least qualitatively reliable for the description of the LLL and first few LLs, say, $n = \pm 1$ LL [28]. This in turn implies that in the analysis of this gap equation, one should use an ultraviolet cutoff Λ of the order of the Landau scale $L(B) \equiv \sqrt{\hbar|eB_\perp|v_F^2/c} \simeq 300\sqrt{B_\perp[\mathrm{T}]}$ [K] (in Kelvin), where $B_\perp$ is the component of $\mathbf{B}$ orthogonal to the graphene plane measured in Tesla. The dimensional coupling constant $G_{\rm int}$ should be taken then as $G_{\rm int} \sim 1/\sqrt{eB_\perp}$ (see below).

Because of the Zeeman term, the $U(4)$ symmetry is broken down to the «flavor» symmetry $U(2)_+ \times U(2)_-$, where the subscript $\pm$ corresponds to up and down spin states, respectively. The generators of the $U(2)_s$, with $s = \pm$, are $I \otimes P_s$, $-i\gamma^3 \otimes P_s$, $\gamma^5 \otimes P_s$, and $\gamma^3\gamma^5 \otimes P_s$ (here I is the 4×4 unit matrix, $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$, and $P_\pm = (1 \pm \sigma^3)/2$ are projectors on spin up and spin down states) [17].

Our goal is searching for solutions of Eq. (3) both with spontaneously broken and unbroken $SU(2)_s$, where $SU(2)_s$ is the largest nonabelian subgroup of the $U(2)_s$. The Dirac mass term $\widetilde{\Delta}_s\overline{\psi}P_s\psi \equiv \widetilde{\Delta}_s\psi^\dagger\gamma^0 P_s\psi$, where $\widetilde{\Delta}_s$ is a Dirac gap (mass), is assigned to the triplet representation of the $SU(2)_s$, and the generation of such a mass would lead to spontaneous flavor $SU(2)_s$ symmetry breaking down to the $\widetilde{U}(1)_s$ with the generator $\gamma^3\gamma^5 \otimes P_s$ [17,24,25]. There is also a Dirac mass term of the form $\Delta_s\overline{\psi}\gamma^3\gamma^5 P_s\psi$ that is a singlet with respect to $SU(2)_s$, and therefore its generation would not break this symmetry. On the other hand, while the triplet mass term is even under time reversal $\mathcal{T}$, the singlet mass term is $\mathcal{T}$-odd (for a recent review of the transformation properties of different mass terms in graphene, see Ref. 29). It is noticeable that consequences of the presence of the mass Δ in graphite were discussed long ago in Ref. 8.

The analysis of gap equation (3) that we use is closely connected with that in Ref. 23 and based on the decomposition of the quasiparticle propagator over the LL poles with the residues expressed through the generalized Laguerre polynomials. A detailed description of the analysis will be presented elsewhere. Here we will describe its main results. It was found that, for a fixed spin, the full inverse quasiparticle propagator takes the following general form (compare with Eq. (2)):

$$iG_s^{-1}(x,y) = [(i\hbar\partial_t + \mu_s + \tilde{\mu}_s\gamma^3\gamma^5)\gamma^0 - \\ - v_F\pi\gamma - \tilde{\Delta}_s + \Delta_s\gamma^3\gamma^5]\delta^3(x-y), \qquad (4)$$

where the parameters μ_s, $\tilde{\mu}_s$, and $\tilde{\Delta}_s$ are determined from gap equation (3). Note that the chemical potential $\mu_\pm$ includes the Zeeman energy $\mp Z$, with $Z = \mu_B B = 0.67B$[T] [K], and the chemical potential $\tilde{\mu}_s$ is related to the density of the conserved pseudospin charge $\psi^\dagger\gamma^3\gamma^5 P_s\psi$, which is assigned to the triplet representation of the $SU(2)_s$. Therefore, while the masses Δ_s and $\tilde{\Delta}_s$ are related to the MC order parameters $\langle\overline{\psi}\gamma^3\gamma^5 P_s\psi\rangle$ and $\langle\overline{\psi}P_s\psi\rangle$, the chemical potentials $\mu_3 \equiv (\mu_+ - \mu_-)/2$ and $\tilde{\mu}_s$ are related to the conventional QHF ones: the spin density $\langle\psi^\dagger\sigma^3\psi\rangle$ and the pseudospin density $\langle\psi^\dagger\gamma^3\gamma^5 P_s\psi\rangle$, respectively. Note that while the triplet Dirac mass term describes the charge density imbalance between the two graphene sublattices [17,24], the pseudospin density describes the charge density imbalance between the two valley points in the Brillouin zone.

The dispersion relations for higher LLs ($|n| \geq 1$) following from Eq. (4) are

$$E_{ns}^{(\sigma)} = -\mu_s + \sigma\tilde{\mu}_s + \\ + \mathrm{sign}(n)\sqrt{2\hbar|neB_\perp|v_F^2/c + (\tilde{\Delta}_s + \sigma\Delta_s)^2}, \qquad (5)$$

where $\sigma = \pm 1$ are connected with eigenvalues of the pseudospin matrix $\gamma^3\gamma^5$. The case of the LLL is special, and its dispersion relation is

$$E_s^{(\sigma)} = -\mu_s + \sigma[\tilde{\mu}_s\,\mathrm{sign}(eB_\perp) + \tilde{\Delta}_s] + \Delta_s\,\mathrm{sign}(eB_\perp). \qquad (6)$$

One can see from Eqs. (5), (6) that at a fixed spin, the terms with σ are responsible for splitting of LLs.

In fact, for each value of spin, our analysis revealed the following three types of solutions: a) a singlet solution with a nonzero singlet mass Δ and with no triplet parameters $\tilde{\Delta}$ and $\tilde{\mu}$, b) a triplet solution with nonzero $\tilde{\Delta}$ and $\tilde{\mu}$, and with the singlet mass Δ being zero, and c) a mixed solution with Δ, $\tilde{\Delta}$, and $\tilde{\mu}$ being nonzero. The latter is realized only in higher LLs. In order to find the most stable solution among them, we compare the free energy density Ω of the corresponding ground states. In the mean field approximation that we use, Ω takes the following form on solutions of the gap equation [30]

$$\Omega VT = i\mathrm{Tr}\left[\mathrm{Ln}\,G^{-1} + \frac{1}{2}(S^{-1}G - 1)\right], \qquad (7)$$

where VT is the space-time volume, the trace, the logarithm, and the product $S^{-1}G$ are taken in the functional sense, and $G = \mathrm{diag}(G_+, G_-)$.

The process of filling the LLs is described by varying the electron chemical potential μ_0. We will consider positive μ_0 (dynamics with negative μ_0 is related by electron-hole symmetry and will not be discussed separately). In this paper we will mostly consider the LLL dynamics (results for the $n = 1$ LL will be briefly described at the end of the paper).

For the case when only the LLL is doped, which corresponds to the condition $|\mu_s \pm \tilde{\mu}_s| \ll L(B)$, we arrive at the following results:

i) A solution with singlet Dirac masses both for spin up and spin down is the most favorable for $0 \leq \mu_0 < 2A + Z$, where $A \equiv G_{\mathrm{int}}|eB_\perp|/8\pi\hbar c$ [31]. It is:

$$\tilde{\Delta}_\pm = \tilde{\mu}_\pm = 0,\ \mu_\pm = \bar{\mu}_\pm \mp A,\ \Delta_\pm = \pm M\,\mathrm{sign}(eB_\perp) \qquad (8)$$

with $\bar{\mu}_\pm \equiv \mu_0 \mp Z$ and $M \equiv A/(1-\lambda)$, $A = \lambda\sqrt{\pi}L^2(B)/2\Lambda$ where the dimensionless coupling constant λ is $\lambda \equiv G_{\mathrm{int}}\Lambda/(4\pi^{3/2}\hbar^2 v_F^2)$ [32]. From dispersion relation (6), we find that $E_+ > 0$ and $E_- < 0$, i.e., the LLL is half filled (the energy spectrum in this solution is σ independent). Therefore the spin gap $\Delta E_0 = E_+ - E_-$ corresponds to the $\nu = 0$ plateau. The value of the gap is $\Delta E_0 = 2M + 2(Z + A)$. It is instructive to compare ΔE_0 with the spin gap in Ref. 16. The latter contains an enhanced Zeeman spin splitting, which corresponds to the second term $2(Z + A)$ in ΔE_0. However, besides this term, there is also the large contribution $2M$ in ΔE_0 in the present solution, which is connected with a dynamical singlet Dirac mass for quasiparticles. The presence of this mass could have important consequences for gapless edge states whose relevance for the physics of the $\nu = 0$ plateau was pointed out in Ref. 33. Generalizing the analysis in Ref. 33, we have found that such states exist only when the full Zeeman splitting $Z + A$ is larger than the Dirac gap $M = A/(1-\lambda)$. This leads to the constraint $Z > \lambda A/(1-\lambda)$. Let us consider the case with $B = B_\perp$. Then, since $Z \sim B_\perp$ and $A \sim \sqrt{B_\perp}$ (see below), this constraint leads to a lower limit $B_\perp^{(\mathrm{cr})}$ for the values of $B_\perp$ at which gapless edge states exist. On the other hand, since Z depends on total B while A depends only on $B_\perp$, adding a longitudinal $B_\parallel$ will decrease the lower limit for $B_\perp$. It would be interesting to check experimentally this point. Also, these features could be relevant for the interpretation of the recent experiments [34], in which no gapless edge states were detected for $B = B_\perp \leq 14$ T. We shall return to this issue below.

ii) A hybrid solution, with a triplet Dirac mass for spin up and a singlet Dirac mass for spin down, is the most favorable for $2A + Z \le \mu_0 < 6A + Z$. It is

$$\widetilde{\Delta}_+ = M,\ \widetilde{\mu}_+ = A\,\mathrm{sign}(eB_\perp),\ \ \mu_+ = \bar{\mu}_+ - 4A,\quad \Delta_+ = 0,$$

$$\widetilde{\Delta}_- = \widetilde{\mu}_- = 0,\ \mu_- = \bar{\mu}_- - 3A,\ \Delta_- = -M\,\mathrm{sign}(eB_\perp). \quad (9)$$

As follows from Eq. (6), while $E_+^{(+1)} > 0$, the energies $E_+^{(-1)}$ and $E_-^{(+1)} = E_-^{(-1)}$ are negative. Consequently, the LLL is now three-quarter filled and, therefore, the gap $\Delta E_1 = E_+^{(+1)} - E_+^{(-1)} = 2(M + A)$ corresponds to the $\nu = 1$ plateau. The latter, unlike the $\nu = 0$ plateau, is directly related to spontaneous $SU(2)_+$ flavor symmetry breaking.

iii) A solution with equal singlet Dirac masses for spin up and spin down states is the most favorable for $\mu_0 > 6A + Z$. It is

$$\widetilde{\Delta}_\pm = \widetilde{\mu}_\pm = 0,\ \ \mu_\pm = \bar{\mu}_\pm - 7A,\ \ \Delta_\pm = -M\,\mathrm{sign}(eB_\perp) \quad (10)$$

(compare with Eq. (8)). It is easy to check from (6) that both E_+ and E_- are negative in this case, i.e., the LLL is completely filled. Therefore, this solution corresponds to the $\nu = 2$ plateau related to the energy gap $\Delta E_2 \simeq \sqrt{2}L(B)$ between the LLL and the $n = 1$ LL.

This analysis leads us to the picture for the LLL plateaus which qualitatively agrees with that in experiments [10,11]. In particular, taking the dimensionless coupling λ to be a free parameter and choosing cutoff Λ to be of the order of the Landau scale $L(B)$, we arrive at the scaling relations, $A \sim \sqrt{|eB_\perp|}$, $M \sim \sqrt{|eB_\perp|}$, and, therefore, $\Delta E_1 = 2(A + M) \sim \sqrt{|eB_\perp|}$ for the gap related to the $\nu = 1$ plateau. One can check that the experimental value $\Delta E_1 \sim 100$ K for $B_\perp = 30$ T [11] corresponds to $\lambda \sim 0.02$. However, because interactions with impurities are ignored in the clean limit used in the present model, it would be more reasonable to consider λ, say, in interval 0.02–0.2. Then, for these values of λ, we find from the constraint $Z > \lambda A/(1-\lambda)$ in the solution i) above that the gapless edge states exist for $|B_\perp| > B_\perp^{(\mathrm{cr})}$, where $0.01\ \mathrm{T} \lesssim B_\perp^{(\mathrm{cr})} \lesssim 200$ T. One can see that $B_\perp^{(\mathrm{cr})}$ is sensitive to the choice of λ. Therefore in order to fix the critical value $B_\perp^{(\mathrm{cr})}$ more accurately, one should utilize a more realistic and constrained model.

As to the $n = 1$ LL, we found that there are the gaps $\Delta E_3 = \Delta E_5 \simeq 2A$ and $\Delta E_4 \simeq 2(Z + A)$ corresponding to the plateaus $\nu = 3$, 5 and $\nu = 4$, respectively (the contributions of Dirac masses are suppressed at least by factor $M^2/L^2(B)$ there). Note that $\Delta E_{3,5}$ and ΔE_4 are essentially smaller than the LLL gaps ΔE_1 and ΔE_0, respectively ($\Delta E_{3,5} \lesssim \Delta E_1/2$). On the other hand, the experimental data yield $\Delta E_4 \simeq 2Z$, and no gaps ΔE_3, ΔE_5 have been observed [10,11]. We believe that a probable explanation of this point is that, unlike Z, the value of the *dynamically* generated parameter A corresponding to the $|n| > 1$ LLs will be essentially reduced if a considerable broadening of higher LLs in a magnetic field is taken into account [17]. If so, the gap ΔE_4 will be reduced to $2Z$ and the gaps ΔE_3, ΔE_5 will become unobservable.

Recently, in Ref. 35, a large width Γ_1 of 400 K was determined for the $n = 1$ LL. The plateaus $\nu = 3$, 5 could become observable if the gaps $\Delta E_3 = \Delta E_5 \simeq 2A$ calculated in the clean limit are at least of order Γ_1 or larger [17]. The LLL gap $\Delta E_1 \simeq 100$ K at $|B_\perp| = 30$ T corresponds to $\Delta E_{3,5} \lesssim 50$ K. Then, taking a conservative estimate $\Gamma_1 = 100$ K and using $A \sim \sqrt{|eB_\perp|}$, we conclude that to observe the $\nu = 3,5$ plateaus, the magnetic fields should be at least as large as $B \sim 100$ T.

In conclusion, we have shown that the QHF and MC order parameters in graphene are two sides of the same coin and they necessarily coexist. This feature could have important dynamical consequences for low energy excitations, in particular, for gapless edge states. It would be desirable to extend the present analysis to a more realistic model setup, including the genuine Coulomb interactions, LLs impurity scattering rates, and temperature.

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