SO(3) symmetry between Néel and ferromagnetic order parameters for graphene in a magnetic field

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I consider the Hubbard model of graphene in an external magnetic field and in the Hartree-Fock approximation. In the continuum limit, the ground-state energy at half filling becomes nearly symmetric under rotations of the three-component vector $\vec{\Delta}=(N_1,N_2,m)$, with the first two components representing the Néel order parameter orthogonal to and the third component the magnetization parallel with the external magnetic field. When the symmetry breaking effects arising from the lattice, Zeeman coupling, and higher Landau levels are included the system develops a quantum critical point at which the antiferromagnetic order disappears and the magnetization has a kink. The observed incompressible states at filling factors ± 1 are argued to arise due to a finite third component of the Néel order parameter at these electron densities. Recent experiments appear consistent with $N_1=N_2=0$ and $N_3\neq 0$, at the filling factors zero and one, respectively.

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I. INTRODUCTION

The nature of the ground state of two-dimensional carbon (i.e., "graphene") in a uniform magnetic field is an issue which has attracted a lot of attention lately. The interest mainly stems from the recent experimental observation[1] of the additional plateaus in the Hall conductivity at the values of zero and unity which are not naturally explained by the picture of noninteracting electrons alone.[2–4] The mechanism behind the formation of the gaps in the energy spectrum that apparently develop within the zeroth Landau level has been a matter of debate. On one hand, the Coulomb repulsion may on general grounds be expected to favor breaking of the sublattice[5] or "valley" symmetry,[6–8] which in the zeroth Landau level are equivalent. If the Zeeman coupling of the electron spin to the magnetic field is entirely neglected the sense of this symmetry breaking can be equal or opposite for the two projections of spin, depending on details of the interaction on the lattice scale. This would yield a staggered pattern of either charge or spin in the ground state, with the concomitant many-body gap in the quasiparticle spectrum.[9] One could, however, also imagine the opposite limit of a strong coupling of the electron spin to the magnetic field, in which the gap in the spectrum at half filling would become essentially a single-particle Zeeman gap. Of course, such a ferromagnetic ground state is already favored by the repulsive Coulomb interaction alone, due to the familiar physics of Hund's rule.[10] The interplay between different possible instabilities in graphene in magnetic field represents an important unsolved problem at the moment.[11,12] Here I would like to point out and explore a surprising symmetry between different order parameters which may help its resolution.

I consider the minimal Hubbard model for the interacting electrons living on a honeycomb lattice. Although admittedly a simplification, the Hubbard model already contains most of the relevant physics. Without a magnetic field it exhibits both the ferromagnetic and antiferromagnetic ground states in its phase diagram,[13] with the latter as stable at half filling.[14] In a field, constraining the Néel vector to lie parallel to it leads to a discontinuous transition between the antiferromagnetic and ferromagnetic ground states at a critical Zeeman coupling, as discussed in the previous work by the author.[9] Here I calculate the ground-state energy in the Hartree-Fock approximation, but for an arbitrary direction of the Néel vector. An immediate, and maybe not entirely unexpected result is that the ground-state energy at half filling is minimized when the Néel order parameter $\vec{N}$ is in fact orthogonal to the external magnetic field. Restricting therefore $\vec{N}$ to its easy plane ($N_3=0$) and taking the magnetization $\vec{m}$ to be parallel to the external magnetic field ($m_1=m_2=0$), the ground state energy at half filling becomes nearly symmetric with respect to an internal SO(3) group of rotations of the three-dimensional order parameter $\vec{\Delta}=(N_1,N_2,m_3)$. This symmetry becomes exact in the zeroth Landau level approximation, if the Zeeman effect and the discreteness of the lattice are also neglected. With these realistic symmetry breaking effects included one finds that with the increase of Zeeman coupling the system at half filling suffers a continuous quantum phase transition from the "mixed" state with both $\vec{N}_\perp\neq 0$ and $m_3\neq 0$ to a pure ferromagnet with $\vec{N}_\perp=0$ and $m_3\neq 0$. This situation is depicted in Fig. 1. With a change in the chemical potential the third Néel component N_3 eventually becomes finite and produces additional incompressible states at the filling factors ± 1. An observation of such, albeit according to our estimate, a rather weak Néel order along the magnetic field at ± 1 would provide a direct support for our theory.

Motivated by a recent experiment,[15] I examine the dependence of the activation gap at filling ± 1 on the in-plane component of the magnetic field, at the fixed perpendicular field. The present theory predicts such a gap to be completely independent of the in-plane component only if at the filling zero $N_\perp=0$ and $m_3\neq 0$, in which case it is simply given by $2N_3$. Given that this seems to be the situation in the experiment, we conclude that for the experimentally relevant values of the parameters the ground state should have a finite N_3 at the filling factor ± 1, whereas it should be a pure ferromagnet at zero filling. This conclusion is in accord with the ob-

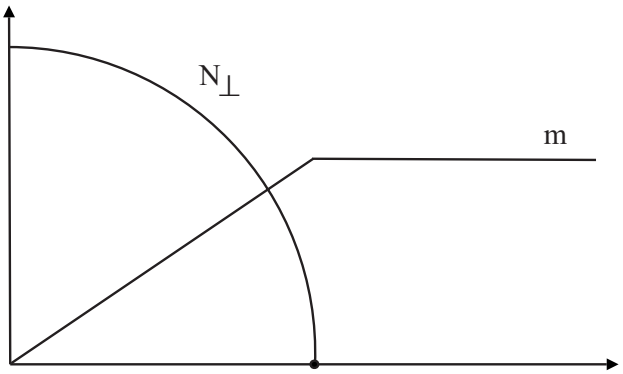

FIG. 1. The dependence of the Néel order parameter ($N_\perp$) orthogonal to and the magnetization (m_3) parallel with the external magnetic field on the Zeeman energy (λ) at the filling factor zero [Eqs. (15)–(18)]. The critical point is located at $\lambda_c=2(g_a-g_f)/(\pi l^2)$, where g_a and g_f are the coupling constants in the Néel and the ferromagnetic channels, respectively. l is the magnetic length.

served dissipative nature of the state at the filling zero, which can be understood in terms of the particular edge-state transport implied by such a ferromagnetic ground state.[16] It is then also in agreement with one of the possible scenarios discussed previously in Ref. 9, where the Néel order parameter was constrained to lie only along the magnetic field.

The paper is organized as follows. In the next section I derive the expression for the ground-state energy of the system as a function of Néel and uniform magnetizations, in the Hartree-Fock approximation. In Sec. III the emergence and the breaking of the approximate SO(3) symmetry by different terms in the Hamiltonian is discussed. The discussion of the result as they pertain to experiment is given in Sec. V. Finally, the main results are summarized in Sec. VI.

II. HARTREE-FOCK GROUND-STATE ENERGY

Let me define the Hubbard model on a honeycomb lattice as H_t+H_U, where

$$H_t=-t\sum_{\vec{A},i,\sigma=\uparrow,\downarrow} u^\dagger_\sigma(\vec{A})v_\sigma(\vec{A}+\vec{b}_i)+\text{H.c.}, \tag{1}$$

and

$$H_U=\frac{U}{16}\sum_{\vec{A}}\{[n(\vec{A})+n(\vec{A}+\vec{b})]^2+[n(\vec{A})-n(\vec{A}+\vec{b})]^2 - [\vec{m}(\vec{A})+\vec{m}(\vec{A}+\vec{b})]^2-[\vec{m}(\vec{A})-\vec{m}(\vec{A}+\vec{b})]^2\}. \tag{2}$$

The sites $\vec{A}$ denote one triangular sublattice of the honeycomb lattice, generated by linear combinations of the basis vectors $\vec{a}_1=(\sqrt{3},-1)(a/2)$, $\vec{a}_2=(0,a)$. The second sublattice is then at $\vec{B}=\vec{A}+\vec{b}$, with $\vec{b}=(1/\sqrt{3},1)(a/2)$. a is the lattice spacing, and $n(\vec{A})=u^\dagger_\sigma(\vec{A})u_\sigma(\vec{A})$ and $\vec{m}(\vec{A})=u^\dagger_\sigma(\vec{A})\vec{\sigma}_{\sigma\sigma'}u_{\sigma'}(\vec{A})$ are the particle number and the magnetization vector at site $\vec{A}$. Variables at the second sublattice are analogously defined in terms of fermion operators $v_\sigma(\vec{B})$. It is easy to check that H_U is just the standard Hubbard on-site repulsion, written here in the rotationally invariant form which will prove to be suitable for our purposes.

Here we are after the Hartree-Fock ground state of the Hubbard model in the uniform magnetic field and at half filling. Even at the highest laboratory fields $\sim$40 T the magnetic length is much larger than the lattice spacing $l\gg a$. It suffices therefore to consider only the continuum theory corresponding to the Hubbard model. General form of the low-energy field theory of graphene has been discussed in detail before.[14] For present purposes it will be enough to consider the Hartree-Fock ground state obtained after the usual decoupling of the interaction term in the ferromagnetic and antiferromagnetic channels. We thus assume a uniform density ($\langle n(\vec{X})\rangle=1,\vec{X}=\vec{A},\vec{B}$), and allow for both the uniform [$\vec{m}=\langle\vec{m}(\vec{A})+\vec{m}(\vec{A}+\vec{b})\rangle$] and staggered magnetizations [$\vec{N}=\langle\vec{m}(\vec{A})-\vec{m}(\vec{A}+\vec{b})\rangle$]. Standard manipulations[17] give the ground-state energy per unit area and at half filling to be

$$E=\frac{\vec{N}^2}{4g_a}+\frac{\vec{m}^2}{4g_f}+E_0[\vec{N},\vec{m}], \tag{3}$$

where E_0 is the ground-state energy per unit area of the resulting single-particle Hamiltonian

$$H_{\text{HF}}=I_2\otimes H_0-(\vec{N}\cdot\vec{\sigma})\otimes\gamma_0+[(\vec{\lambda}+\vec{m})\cdot\vec{\sigma}]\otimes I_4. \tag{4}$$

$\vec{\lambda}=g_Z\vec{B}$ represents the Zeeman effect of the uniform magnetic field $\vec{B}$, and g_Z is the electron g factor. $H_0=i\gamma_0\gamma_i(-i\partial_i-A_i)$, with $B=\epsilon_{3ij}\partial_iA_j$, is the standard Dirac Hamiltonian near the two Fermi points in the spectrum of H_t.[18,19] For simplicity, the magnetic field will be assumed to be orthogonal to the graphene plane, until further notice. We work in "graphene representation" of the Clifford algebra[14] in which $\gamma_0=I_2\otimes\sigma_3$, $\gamma_1=\sigma_3\otimes\sigma_2$, $\gamma_2=-I_2\otimes\sigma_1$, where $\{I_2,\vec{\sigma}\}$ is the standard Pauli basis of two-dimensional matrices. Likewise, I_4 represents the four-dimensional unit matrix. In our units $\hbar=e/c=v_F=1$. The coupling constants g_f and g_a are both proportional to the original repulsion energy U, and positive. Although they are exactly equal at the lattice scale, as evident from the form of H_U in Eq. (2), they in general will not be in the effective linearized Dirac theory sensible only below a certain momentum cutoff Λ. Subscribing to the usual logic of the low-energy description, g_f and g_a must be considered only as effective parameters which themselves depend on the cutoff Λ in a way that ensures the cutoff independence of all physical quantities. This observation will play a role in the selection of the ground state, as will be discussed shortly.

To proceed one needs the spectrum of the eight-dimensional Hamiltonian H_{HF}. Perhaps this is most easily computed by casting it into a block-diagonal form $H_{\text{HF}}=H_1\oplus H_2$,[20] with

$$H_{1(2)} = \pm I_2 \otimes \sigma_1(-i\partial_1 - A_1) - I_2 \otimes \sigma_2(-i\partial_2 - A_2) - (\vec{N}\cdot\vec{\sigma}) \otimes \sigma_3 + (\lambda + m_3)\sigma_3 \otimes I_2. \quad (5)$$

Here we have chosen the third spin axis and the magnetization to be along the magnetic field, i.e., $m_1 = m_2 = 0$, $m_3 > 0$. Next we note that $H_1 = U_1^\dagger H U_1$, with $U_1 = I_2 \oplus i\sigma_2$, and

$$H = H_0 + iN_1\gamma_0\gamma_3 + iN_2\gamma_0\gamma_5 - N_3\gamma_0 + i(\lambda + m_3)\gamma_3\gamma_5 \quad (6)$$

and $\gamma_3 = \sigma_1 \otimes \sigma_2$, $\gamma_5 = \sigma_2 \otimes \sigma_2$. Similarly, $H_2 = U_2^\dagger H U_2$, with $U_2 = i\sigma_2 \oplus I_2$, with $N_3 \to -N_3$. It is sufficient therefore to find the spectrum of the single four-dimensional Hamiltonian H. After some algebra the eigenvalues of H_{HF} are this way found at $\pm e_{n\sigma}$ with

$$e_{n\sigma} = \{N_\perp^2 + [(N_3^2 + 2nB)^{1/2} + \sigma(\lambda + m_3)]^2\}^{1/2}, \quad (7)$$

with $\sigma = \pm 1$, $\vec{N}_\perp = (N_1, N_2)$, and the degeneracies per unit area of $1/(\pi l^2)$ and $1/(2\pi l^2)$, for $n = 1, 2, 3, \ldots$, and $n = 0$, respectively. Note that for $\vec{N} = 0$ the eigenvalues become the familiar relativistic Landau levels split by the Zeeman term, as expected. For $\lambda + m_3 = 0$, on the other hand, the spectrum reduces to the Landau levels of the massive Dirac Hamiltonian, with the mass $|\vec{N}|$, also in agreement with the previous calculations.[9]

At half filling then the ground state of H_{HF} has all the eigenstates with negative energies filled, and all the others empty, so

$$E_0[\vec{N}, m_3] = -\frac{1}{2\pi l^2}\sum_{\sigma=\pm 1}\left[e_{0\sigma} + 2\sum_{n\neq 0} e_{n\sigma}\right]. \quad (8)$$

The variational Hartree-Fock ground-state energy is then determined by the least value of the expression in Eq. (3).

III. SO(3) SYMMETRY AND ITS BREAKING

Let us minimize the Hartree-Fock ground state energy given by Eqs. (3) and (8), assuming $\lambda \neq 0$. Choosing $|\vec{N}|$ and N_3 as independent variables and then differentiating with respect to N_3 yields

$$\sum_{\sigma=\pm 1} \sigma(\lambda + m_3)\left[\frac{1}{e_{0\sigma}} + \sum_{n\neq 0}\frac{2}{e_{n\sigma}}\frac{N_3}{\sqrt{N_3^2 + 2nB}}\right] = 0. \quad (9)$$

The left-hand side of the equation vanishes for $N_3 = 0$, and otherwise is a negative definite function of N_3. $N_3 = 0$ is therefore the only solution. One can also show that this solution represents the minimum of the energy. Restricting the Néel vector then to be orthogonal to the magnetic field the ground-state energy in Eq. (3) can be rewritten as

$$E = E_{\mathrm{SO}(3)} + E', \quad (10)$$

where

$$E_{\mathrm{SO}(3)} = \frac{\vec{N}_\perp^2 + m_3^2}{4g_a} - \frac{1}{\pi l^2}(\vec{N}_\perp^2 + m_3^2)^{1/2}, \quad (11)$$

and $E' = E_\Lambda + E_Z + E_{HLL}$, with

$$E_\Lambda = \frac{(g_a - g_f)}{4g_f g_a} m_3^2, \quad (12)$$

$$E_Z = \frac{1}{\pi l^2}\{(\vec{N}_\perp^2 + m_3^2)^{1/2} - [\vec{N}_\perp^2 + (\lambda + m_3)^2]^{1/2}\}, \quad (13)$$

$$E_{HLL} = -\sum_{\sigma=\pm 1}\sum_{n=1}^{M}\frac{\{\vec{N}_\perp^2 + [(2nB)^{1/2} + \sigma(\lambda + m_3)]^2\}^{1/2}}{\pi l^2}. \quad (14)$$

This form makes it manifest that the Hartree-Fock ground-state energy at half filling is nearly symmetric with respect to rotations of the three-component order parameter $\vec{\Delta} = (N_1, N_2, m_3)$. The identification of this approximate internal SO(3) symmetry is our central result. The SO(3) symmetry is in the Hubbard model broken by three terms of different physical origin: (1) the difference between the coupling constants g_a and g_m at the cutoff Λ (E_Λ), (2) the finite Zeeman coupling to the magnetic field λ (E_Z), and (3) the $n \neq 0$ Landau level contribution (E_{HLL}). If one were to consider only the zeroth Landau level, use the bare values of the couplings for which $g_a = g_m$, and neglect the Zeeman coupling, the Hartree-Fock ground-state energy would become perfectly SO(3) symmetric. In particular, the antiferromagnetic state with the Néel vector orthogonal to the external magnetic field and the ferromagnetic state with the magnetization along the same field would in this approximation appear as degenerate.

Clearly, the Zeeman term favors magnetization. Similarly, it can be shown that H_{HLL} prefers the Néel components.[21] It is less obvious what the sign of the "easy-axis anisotropy," i.e., of $g_a - g_f$, in E_Λ should be. This is determined by the flow of the two coupling constants as the high-energy modes between the momenta $\sim 1/l$ and $\sim 1/a$ are integrated out essentially at zero magnetic field. Since the leading instability of the Hubbard model on a honeycomb lattice and at half filling as the interaction strength is increased is towards the antiferromagnetism, we may assume that in general $g_a > g_f$ in the low-energy theory. This would also be in accord with the explicit renormalization group calculation for weak couplings.[14]

The ground state in the Hartree-Fock approximation is thus the result of the competition between the high-energy modes represented by H_Λ and H_{HLL}, and the Zeeman coupling, which favor antiferromagnetic and ferromagnetic solutions, respectively. Since the effect of H_{HLL} is in the same direction as of H_Λ, to keep the algebra simple we will drop H_{HLL} altogether and just assume $g_a - g_f > 0$ in the Eq. (10). This is a particularly good approximation at the laboratory magnetic fields at which the inclusion of the higher Landau levels is expected to provide corrections to our results of higher order in the small parameter a/l. Minimizing the energy in Eq. (10), for $\lambda < \lambda_c$ we then find

$$|\vec{N}_\perp| = \frac{g_a}{g_a - g_f}\sqrt{\lambda_c^2 - \lambda^2}, \quad (15)$$

$$m = \frac{g_f}{g_a - g_f}\lambda, \quad (16)$$

and for $\lambda > \lambda_c$,

$$\vec{N}_\perp = 0, \tag{17}$$

$$m = \frac{g_f}{g_a - g_f}\lambda_c, \tag{18}$$

where $\lambda_c = 2(g_a - g_f)/(\pi l^2)$. With the increase of the Zeeman coupling there is a continuous transition at which the Néel order disappears, and the magnetization saturates to its maximum (Fig. 1).

Note that if the Néel vector is constrained to be along the magnetic field, so that $\vec{N}_\perp = 0$, the above quantum critical point becomes replaced with the level crossing between the purely antiferromagnetic ($N_3 \neq 0$, $m_3 = 0$) and purely ferromagnetic ($N_3 = 0$, $m_3 \neq 0$) ground states.[9] Such a pure antiferromagnet would correspond to a local maximum of the energy in Eq. (3), however. It seems always energetically favorable to compromise between the two competing magnetic orderings by orienting the Néel vector orthogonally to the field.

IV. DISCUSSION

While it is not *a priori* clear at which side of the transition should the experimental samples lie at half filling, increasing sufficiently the component of the magnetic field parallel to the graphene layer should always place the system into the purely ferromagnetic state. The experimental fact that the system at the filling factor zero is dissipative suggests that this is probably already the case even for the magnetic field completely orthogonal to the graphene's plane.[16] Spin splitting as the origin of the measured gap at half filling has also been suggested very recently in Ref. 15. Most importantly, the experiment of Jiang *et al.* offers compelling evidence that the gap at filling factor ±1 is independent of the total magnetic field, and thus likely to be a consequence of interactions.[15] And this is precisely what follows from our theory.[9] When the chemical potential gets close to the energy of the first excited states laying at

$$\mu_c = \pm\sqrt{\vec{N}_\perp^2 + (\lambda + m_3)^2}, \tag{19}$$

the Hartree-Fock ground-state energy may always be lowered by developing a finite third Néel component N_3. This pushes half of the states in question below the chemical potential and opens a gap. This way an incompressible state at filling factors ±1 would be formed irrespectively of whether $\vec{N}_\perp$ was zero or finite at the filling factor zero. Note, however, that the Eq. (7) implies that this mechanism is operative only in the $n=0$ Landau level; the states belonging to the other Landau levels do not get split but only shifted in energy when $N_3 \neq 0$. Consequently, at weak coupling N_3 will become finite only in the ±1 state and otherwise not. The incompressible states that follow from the inclusion of a finite chemical potential into Eq. (3) lie therefore only at filling factors 0, ±1, and all even integers.

Let us assume therefore a weak third Néel component N_3 at the filling factor ±1. The activation gap at this filling then becomes

$$E_{\text{gap}} = \frac{2(\lambda + m_3)}{[N_\perp^2 + (\lambda + m_3)^2]^{1/2}} N_3 + O(N_3^2). \tag{20}$$

For a small Zeeman term $\lambda < \lambda_c$, Eqs. (15) and (16) give then

$$E_{\text{gap}} = \frac{2\lambda}{\lambda_c} N_3 + O(N_3^2), \tag{21}$$

whereas when $\lambda > \lambda_c$ and $N_\perp = 0$,

$$E_{\text{gap}} = 2N_3 + O(N_3^2). \tag{22}$$

Recalling that both $N_3 \sim B_\perp$ and $\lambda_c \sim B_\perp$, whereas $\lambda \sim B$, where B is the total and $B_\perp$ the perpendicular component of the magnetic field, we see that the gap is independent of the field's in-plane component *only* in the latter case. The experiment is therefore consistent with $N_3 \neq 0$ at the filling factor ±1, and with $N_\perp = 0$ at the filling factor zero. This may not be very surprising in view of the equality between the couplings g_a and g_f at the lattice scale, which makes the critical Zeeman coupling λ_c likely to be exceeded by the experimental value of λ.[22]

Finally, restoring a finite range to electron-electron interactions may replace the antiferromagnetic ground state discussed here with a charge density wave with the particle density alternating (around the value of unity) on the two sublattices. In this case the mean field phase diagram would remain the same as discussed previously in Ref. 9. Provided that the on-site repulsion is indeed the dominant effect of the Coulomb interaction in graphene, our prediction is that at filling factors ±1 and at magnetic fields $B \sim 10T$ the system has a weak Néel component $N_3 \sim (a/l)^2 \mu_B \sim (10^{-3} - 10^{-4})\mu_B$ per electron. μ_B is the Bohr magneton. The inherent weakness of the Néel order derives from a small fraction of electrons occupying the relevant $n=0$ Landau level, which is the sole source of antiferromagnetism in this case. The existence of such ordering at the fillings ±1 can be used to distinguish the present proposal from all others in the current literature on the subject.

V. SUMMARY

To summarize, the ground-state energy in the Hartree-Fock approximation to the Hubbard model on honeycomb lattice and at half filling is nearly symmetric with respect to rotations between the components of the Néel order orthogonal to and the magnetization parallel with the external magnetic field. The effects of the symmetry breaking terms originating from discreetness of the lattice, Zeeman interaction, and $n \neq 0$ Landau levels were examined. It was shown that whereas the component of the Néel order parameter parallel to the magnetic field always vanishes at half filling, it becomes finite (only) at filling factors ±1, introducing this way a gap in the spectrum. The existence of such a weak Néel order along the magnetic field $\sim 10^{-4}\mu_B$ per electron is proposed as a litmus test of the present theory.

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[22] Note that when $N_\perp = 0$ the activation gap at zero filling is $2(\lambda + m_3)$, and thus, as demanded by its observed magnitude, significantly enhanced by the interactions.