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Novel Electric Field Effects on Landau Levels in Graphene

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A new effect in graphene in the presence of crossed uniform electric and magnetic fields is predicted. Landau levels are shown to be modified in an unexpected fashion by the electric field, leading to a collapse of the spectrum, when the value of electric to magnetic field ratio exceeds a certain critical value. Our theoretical results, strikingly different from the standard 2D electron gas, are explained using a "Lorentz boost," and as an "instability of a relativistic quantum field vacuum." It is a remarkable case of emergent relativistic type phenomena in nonrelativistic graphene. We also discuss few possible experimental consequence.

Graphene has been in the forefront of nanoelectronics and quantum condensed matter physics over the last couple of years. The mechanical rigidity, being able to peel off single graphene layer [1] and the ability to make electrical contacts has made the system very appealing from building devices and experimental points of view [2,3]. One of the remarkable discoveries in graphene is the anomalous 2D quantized Hall effect. A variety of rich physics and anomalous phenomena are tied to a remarkable "relativisticlike" spectrum that electron and holes possess in graphene [4,5]. This has made graphene important and interesting from several points of view in physics.

In the present Letter, we investigate the effect of a uniform electric field, applied along the graphene sheet, on its already anomalous Landau level spectrum. We find that, within the low energy approximation near the Fermi surface (Dirac points), the problem can be exactly solved. We find strikingly new effects of electric field on the Landau levels which is different from the Landau levels of standard 2D electron gas.

We find that the Landau spectrum gets scaled, for a given k_y quantum number, by an electric field dependent dimensionless parameter ($\beta = \frac{E}{v_F B}$). As the value of this parameter is increased, spacings between the Landau levels decrease. This Landau level contraction is a consequence of electric field induced quantum mechanical mixing of Landau levels. The entire Landau level structure collapses at a critical value of this parameter. Further, the "relativistic" character of the spectrum (with Fermi velocity replacing the velocity of light), leads to a novel interpretation of our result in terms of relativistic boosts and the mixing of electric and magnetic fields in moving frames of reference. We confirm our analytical result by solving the full tight binding model for a graphene sheet in the presence of magnetic and electric fields numerically. The collapse seen in the low energy approximation, is indeed accelerated in the actual tight binding model.

The modified wave functions and energy spectrum will have implications on the nature of quantum Hall breakdown. We briefly touch upon this issue at the end, and point

out how it could be different from the standard quantum Hall breakdown.

Electronic states of graphene are well described by the tight binding Hamiltonian for the π electrons of the carbon atoms. In graphene, the carbon atoms form a triangular lattice with a basis of two geometrically inequivalent atoms placed $a/\sqrt{3}$ apart, where $a = 2.456A^0$ is the lattice constant. The overlap integral between the nearest carbon atoms is $t \approx 2.71$ eV. We denote the triangular lattice sites by $\mathbf{R}_i = i_1\hat{\mathbf{e}}_1 + i_2\hat{\mathbf{e}}_2$, where $\hat{\mathbf{e}}_1 = \hat{\mathbf{x}}$ and $\hat{\mathbf{e}}_2 = -\frac{1}{2}\hat{\mathbf{x}} + (\sqrt{3}/2)\hat{\mathbf{y}}$ are the basis vectors. $c_{\mathbf{i}r\sigma}$ ($r = 1, 2$, and $\sigma = \uparrow, \downarrow$) represent the electron annihilation operators with sublattice index r and spin index σ at $\mathbf{R}_i$. The Hamiltonian is then written as

$$H = -t\sum_{\mathbf{i}\sigma} c^{\dagger}_{\mathbf{i}2\sigma}(c_{\mathbf{i}1\sigma} + c_{\mathbf{i}+\hat{\mathbf{e}}_2 1\sigma} + c_{\mathbf{i}-\hat{\mathbf{e}}_3 1\sigma}) + \text{H.c.}, \quad (1)$$

where $\hat{\mathbf{e}}_3 = -(\hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_2)$. The electronic dispersion for graphene has two points in a Brillouin zone which separate the positive and negative energy eigenstates. These so-called Dirac points are $K_{1,2} = \pm \frac{2\pi}{a}[(1/\sqrt{3})\hat{\mathbf{x}} + \hat{\mathbf{y}}]$. The dispersion relation in the proximity of the Dirac points is linearly proportional to $|\mathbf{k}|$. The low energy modes around these points are described by slowly varying fields $\psi_{r\eta\sigma}(\mathbf{R}_i)$ defined as

$$c_{ir\sigma} = e^{i\mathbf{K}_1\cdot\mathbf{R}_i}\alpha^z_{rr'}\psi_{r'1\sigma}(\mathbf{R}_i) + e^{i\mathbf{K}_2\cdot\mathbf{R}_i}\alpha^x_{rr'}\psi_{r'2\sigma}(\mathbf{R}_i) \quad (2)$$

where α^x, α^y are the Pauli matrices. The effective Hamiltonian for the low energy modes is the Dirac Hamiltonian.

$$H = v_F \int d^2x \sum_{\eta\sigma} \Psi^{\dagger}_{\eta\sigma}\boldsymbol{\alpha}\cdot\mathbf{p}\Psi_{\eta\sigma}, \quad (3)$$

where $v_F = (\sqrt{3}/2)\frac{at}{\hbar}$ is the Fermi velocity. $\Psi_{\eta\sigma}$ are two component field operators where η ($= 1, 2$) is the valley index, corresponds to two Dirac points and σ ($= \uparrow, \downarrow$) is the spin index. The spectrum can be obtained by solving the one particle equation to get the linear dispersion, $\epsilon(\mathbf{k}) = \pm\hbar v_F|\mathbf{k}|$. In the presence of an external magnetic

field perpendicular to the graphene plane the one particle Hamiltonian, $h = v_F \boldsymbol{\alpha} \cdot \boldsymbol{\Pi}$, where $\boldsymbol{\Pi} = \mathbf{p} + e\mathbf{A}$, The energy eigenvalues are

$$\epsilon_{n,k_y} = \mathrm{sgn}(n)\sqrt{2|n|}\frac{\hbar v_F}{l_c} \quad (4)$$

n is the Landau level index, $k_y = \frac{2\pi}{L_y}l$ is the quantum number corresponding to translation symmetry along y axis, both n and l are integers [we choose Landau gauge $\mathbf{A}(\mathbf{r}) = xB\hat{\mathbf{y}}$] and $l_c = \sqrt{\hbar/eB}$ is the magnetic length. Unlike the case of the nonrelativistic electron in a magnetic field, where the spectrum has a linear dependence on the magnetic field and the non-negative integer valued Landau level index, the graphene Landau levels have a square root dependence on both magnetic field and Landau level index. The degeneracy of each level is given by the number of magnetic flux quanta passing through the sample. The eigenfunctions are

$$\psi_{nk_y}(x, y) \propto e^{ik_y y}\begin{pmatrix} \mathrm{sgn}(n)\phi_{|n|-1}(\xi) \\ i\phi_{|n|}(\xi) \end{pmatrix} \quad (5)$$

where $\phi_n(\xi)$ are the harmonic oscillator eigenfunctions and $\xi \equiv \frac{1}{l_c}(x + l_c^2 k_y)$.

We now consider the above system in the presence of a constant electric field in the x direction. The single particle Hamiltonian is then given by

$$h = v_F \boldsymbol{\alpha} \cdot \boldsymbol{\Pi} + \mathbf{1}eEx. \quad (6)$$

The Lorentz covariant structure of the Hamiltonian, with v_F playing the role of the speed of light, can be used to solve it exactly [6]. It is known from special relativity, if $v_F B > |\mathbf{E}|$, then we can always boost to a frame of reference where the electric field vanishes and the magnetic field is reduced. We can then use the solution in Eq. (4) and boost back to get the exact spectrum of the Hamiltonian in Eq. (6). Here the boost transformation amounts to doing a transformation on the space-time coordinate system. To implement the above procedure, it is convenient to work with the manifestly covariant time dependent Dirac equation,

$$i\hbar\gamma^\mu\left(\partial_\mu + i\frac{e}{\hbar}A_\mu\right)\Psi(x^\mu) = 0 \quad (7)$$

where $x^0 = v_F t$, $x^1 = x$, $x^2 = y$, $\gamma^0 = \alpha^z$, $\gamma^1 = i\alpha^y$, $\gamma^2 = -i\alpha^x$, $\partial_\mu = \frac{\partial}{\partial x^\mu}$. $A^0 = \phi$, the scalar potential, $A^1 = A_x$, $A^2 = A_y$, and $\Psi(x^\mu)$ is a two component spinor. We now apply a Lorentz boost in the y direction (perpendicular to the electric field),

$$\begin{pmatrix} \tilde{x}^0 \\ \tilde{x}^2 \end{pmatrix} = \begin{pmatrix} \cosh\theta & \sinh\theta \\ \sinh\theta & \cosh\theta \end{pmatrix}\begin{pmatrix} x^0 \\ x^2 \end{pmatrix} \quad (8)$$

and $\tilde{x}^1 = x^1$. The wave function transforms, $\tilde{\Psi}(\tilde{x}^\mu) = e^{(\theta/2)\alpha_y}\Psi(x^\mu)$. Applying the above transformations and choosing $\tanh\theta = \frac{E}{v_F B} = \beta$, we can rewrite the Dirac equation in Eq. (7),

$$\left[\gamma^0\tilde{\partial}_0 + \gamma^1\tilde{\partial}_1 + \gamma^2\left(\tilde{\partial}_2 + \frac{i}{l_c^2}\sqrt{1 - \beta^2}\tilde{x}^1\right)\right]\tilde{\Psi}(\tilde{x}^\mu) = 0. \quad (9)$$

In the boosted coordinates, where $|\beta| < 1$, it is a problem of a Dirac electron in a (reduced) magnetic field, $\tilde{B} = B\sqrt{1 - \beta^2}$. The time component of the 3-momentum in the boosted frame, $\tilde{\epsilon}_{n,\tilde{k}_y} = \mathrm{sgn}(n)\sqrt{2|n|}\frac{\hbar v_F}{l_c}(1 - \beta^2)^{1/4}$ is not the physical energy eigenvalue of our problem. We have to apply the inverse boost transformation to obtain the spectrum and eigenfunctions of our problem,

$$\epsilon_{n,k_y} = \mathrm{sgn}(n)\sqrt{2|n|}\frac{\hbar v_F}{l_c}(1 - \beta^2)^{3/4} - \hbar v_F \beta k_y, \quad (10)$$

$$\Psi_{n,k_y}(x, y) \propto e^{ik_y y}e^{-(\theta/2)\alpha_y}\begin{pmatrix} \mathrm{sgn}(n)\phi_{|n|-1}(\xi') \\ i\phi_{|n|}(\xi') \end{pmatrix}, \quad (11)$$

$$\xi' \equiv \frac{(1 - \beta^2)^{1/4}}{l_c}\left(x + l_c^2 k_y + \mathrm{sgn}(n)\frac{\sqrt{2|n|}l_c\beta}{(1 - \beta^2)^{1/4}}\right). \quad (12)$$

The energy eigenvalues of the standard 2D electron gas in crossed magnetic and electric fields are given by $\epsilon_{n,k_y} = (n + \frac{1}{2})\hbar\omega_c - \hbar k_y\frac{E}{B} - \frac{m}{2}(\frac{E}{B})^2$. The main difference between the two besides the $\sqrt{n}$ and $\sqrt{B}$ dependence, is that the low lying graphene Landau level spacing scales as $(1 - \beta^2)^{3/4}$, whereas the spacing is independent of the electric field in the nonrelativistic case. Comparing the eigenfunctions with and without the electric field (5) and (11), we see that the effect of the electric field is to (un)squeeze the oscillator states as well as to mix the particle and hole wave functions. Squeezing corresponds to the change in l_c and the eigenfunctions in Eq. (11) can be expanded as superposition of states in Eq. (5). Thus, unlike in the usual semiconductor samples, in graphene the electric field causes Landau level mixing. Also notice in (12) that the location of the Gaussian also shifts as a function of the Landau level index n, unlike the standard 2D electron gas.

As β approaches unity, from Eq. (12) we infer that, to keep the Gaussian shifts within the linear extent of the system requires larger values of k_y, which takes us beyond the long wavelength approximation. Moreover the Eq. (10) hands a collapse of the Landau level spectrum at $\beta = 1$. One may wonder if the collapse we have found is an artifact of the low energy approximation? Interestingly, we find that in our full tight binding calculation the collapse persists, and in fact it occurs at a value of β even smaller than unity.

We have performed extensive numerical computations on the tight binding model for graphene with magnetic and electric fields, using lattice sizes ranging from 60×60 to 600×600. The magnetic field enters through the Peierls substitution, $t \to te^{i(2\pi e/\hbar)\int \mathbf{A}\cdot d\mathbf{l}}$ in Eq. (1). $\mathbf{A}(\mathbf{r})$ is chosen in such a way that the contribution to the phase term comes from hopping along one of the three bonds for each carbon

atom. This enables us to maintain translation symmetry along the $\hat{\mathbf{e}}_2$ axis of the triangular lattice. The problem then reduces to the 1D Harper equation.

$$\epsilon\phi_{1,n_1} = 2t\cos\left(\frac{k_2a + n_1\varphi}{2}\right)\phi_{2,n_1} + t\phi_{2,n_1+1},$$

$$\epsilon\phi_{2,n_1} = 2t\cos\left(\frac{k_2a + n_1\varphi}{2}\right)\phi_{1,n_1} + t\phi_{1,n_1-1}. \quad (13)$$

Here φ is the magnetic flux passing through each plaquette, k_2 is the wave vector, and n_1 is the $\hat{\mathbf{e}}_1$ component of triangular lattice coordinate.

We choose the value of the magnetic field such that $L \gg l_c \gg a$, where L is the linear extent of the system. The condition $l_c \gg a$ ensures that we stay away from the Hofstadter butterfly kind of commensurability effects on the spectrum, and $L \gg l_c$ ensures that a large number of cyclotron orbits fit in the sample. For our numerics, we expressed all energies in units of t and all lengths in units of a.

Figure 1 shows the results of our numerical investigation for zero and Fig. 2 for a finite ($\beta = 0.1$) electric field. Figure 1 shows the spectrum at low energies and the eigenvalues that are constant with respect to k_y are the Landau levels. They have $\sqrt{n}$ behavior and are in excellent agreement with the analytical result and the eigenstates that vary with k_y are the chiral edge states responsible for the quantum Hall current. In our numerics the lattice has zigzag edges at the two ends along $\hat{\mathbf{e}}_1$. It is well known that the zigzag edges result in zero-eigenvalue states even in the absence of external magnetic field [7]. These zero-eigenvalues surface states which are localized at the
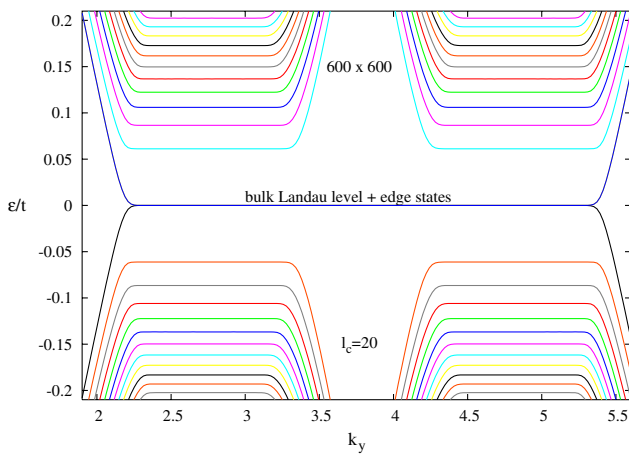
boundary and $n = 0$ Landau level forms degenerate set of states as shown in Fig. 1. However, Fig. 2 shows that this degeneracy gets lifted in the presence of an electric field. For small electric fields the wave function of these edge states continues to be localized near the edge of the sample. Any difference in eigenvalues of these surface states is because of the potential seen by them due to the externally applied electric field at the two edges of the sample. A characteristic feature of these edge states is that they do not vary with the wave vector, whereas the Landau levels develop a linear k_y dependence with electric field.

Figure 3(b), shows $\sqrt{n}$ scaling of Landau levels for a given k_y value. For zero electric field we see an excellent match between analytics and numerics. And for the case of finite electric fields we see a systematic deviation from exact results as we suspected from our exact result. As $\beta \to 1$, the tight binding results shows a faster collapse. Figure 3(a) shows the collapse has already occurred at $\beta = 0.9$, near one the Dirac points.

We show below that one of the consequences of the Landau level contraction (10) and the n dependent Gaussian shift (12) is the possibility of a "dielectric breakdown," which is different from the conventional ones. The single particle spectrum and states we have obtained thus far (for a given E and B) can be used to construct stable many-body quantum Hall ground states. However, the external electric field not only modifies the single particle wave function and spectrum, but can also destabilize the ground state through spontaneous creation of particle-hole pairs, i.e., by a dielectric breakdown. We present a simple
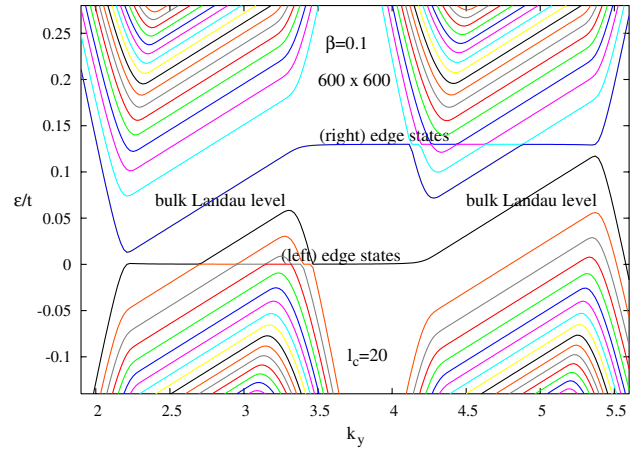

FIG. 1 (color online). Energy eigenvalues ϵ_{n,k_y}, for electrons in graphene computed from the tight binding model for a hexagonal lattice subjected to a magnetic field $B = 27.3$ T (or $l_c = 20a$ where a is the triangular lattice spacing) for a system size of $600a \times 600a$. The plot shows ϵ_{n,k_y} in the units of t as function of k_y, where k_y is the wave vector in the y direction. Two sets of horizontal lines are Landau levels corresponding to the two valleys and $n = 0$ Landau level and the edge states are degenerate.

FIG. 2 (color online). Energy eigenvalues ϵ_{n,k_y} for electrons computed for the tight binding model for parameters given in Fig. 1 and an external electric field E applied along x axis, given by the parameter $\beta = \frac{E}{v_F B} = 0.1$. The electric field gives a linear k_y dependence to the bulk Landau levels whereas it gives a constant shift to the edge states. The part of solid line labeled "bulk Landau level" are $n = 0$ Landau levels and parallel lines above and below them are Landau levels corresponding to positive and negative n respectively. Set of points parallel to k_y labeled "edge states" are surface states localized at the zigzag boundary.
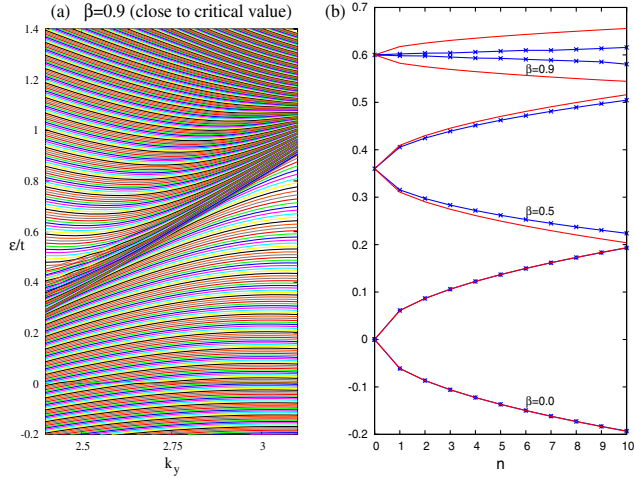
FIG. 3 (color online).   (a) shows the energy eigenvalues around the Dirac point plotted as function of k_y for $\beta = 0.9$. The collapse can be clearly seen (b) shows the modulus of the eigenvalues $|\epsilon_{n,k_y}|$ for a value of $k_y = 2.785$ computed from the tight binding model for system size $600a \times 600a$, magnetic field $B = 27.3$ T or $l_c = 20a$, electric field given by parameter $\beta = 0.0, 0.5, 0.9$, plotted as a function of n.

formula for dielectric breakdown, without giving full details. It has an unusual dependence on the length scale over which the potential fluctuates and on the Landau level index n. This peculiar feature is absent in standard quantum 2D electron systems [8]. Specifically, we find that for slowly varying electric field fluctuations over a length scale ℓ_E and for large Landau level index, the critical voltage for breakdown is given by

$$V_c \approx \frac{\Delta_n(0, B)}{e}\left[1 \pm \kappa n\left(\frac{l_c}{\ell_E}\right)^2\right], \qquad (14)$$

where κ is a constant of the order of unity, which depends on the strength of the electric field fluctuations and Δ_n is gap between levels n and $n + 1$. This means that if we have an electric field, nonuniform over a nanoscopic scale ($\ell_E \sim l_c$), it will cause local breakdown even before the critical field is reached. Such situations can be created through in-plane or out-of-plane charged impurities or STM tips, in addition to external electric fields. It is interesting that such an anomalous local breakdown is Landau level index n dependent, we expect that the quantum Hall breakdown should be qualitatively different for $n = 0$ and $n \neq 0$ within graphene.

In the light of new spectroscopic experiments [9], we claim that the contraction in Landau level spacing and the collapse can be observed at fields attainable in laboratories. The gap between $n = 0$ and $n = 1$ for $B \sim 1$ T is ~ 35 meV, for $E \sim 3 \times 10^5$ V m^{-1}, 10% reduction in the gap is expected. And the collapse of the Landau levels should also be observable by applying $E \sim 10^6$ V m^{-1}. In the context of quantum Hall breakdown, the dependence of critical voltage on ℓ_E as given in Eq. (14) suggests that the

breakdown phenomena should be different from what we observe in standard 2D quantum Hall system. Moreover graphene's Landau level index dependence on V_c, we expect the breakdown phenomena is going to be different for $n \neq 0$ from that of $n = 0$.

It will be interesting to study graphene from the point of view of the present Letter. As quantum Hall phenomena are beginning to be seen in pyrolytic graphite [10] and possibly in carbon eggshells [11], it will be very interesting to study electric field effects in these systems as well, to confirm our predictions.

In summary, we have made a theoretical prediction of a remarkable phenomena in graphene: Landau level contraction and an eventual collapse, induced by crossed electric fields. The local dielectric breakdown has a peculiar length and Landau level index dependence. These phenomena, not known in the standard 2D electron gas, is a consequence of the relativistic type spectrum of low energy electrons and holes in graphene.

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