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Nonlinear transverse current response in zigzag graphene nanoribbons

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By employing a self-consistent approach, we reveal a number of unique properties of zigzag graphene nanoribbons under crossed electric and magnetic fields: (1) a very strong electrical polarization along the transverse direction of the ribbon, and (2) a strong nonlinear Hall current under a rather moderate electrical field. At the field strength of 5000 V/cm, the ratio of the nonlinear current to the linear current is around 1 under an applied magnetic field of 7.9 T. Our results suggest that graphene nanoribbons are an ideal system to achieve a large electrical polarizability. Our results also suggest that the nonlinear effect in graphene nanoribbons has been grossly underestimated without the self-consistent scheme proposed here. © 2011 American Institute of Physics. [doi:10.1063/1.3647783]

Since its synthesis in 2004,¹ graphene has become one of the focal points in the low-dimensional condensed matter physics.^{1–4} The physical properties of graphene-related material have been extensively studied. Many novel properties have been experimentally verified, such as the electron-hole symmetry, the odd-integer quantum Hall effect,^{3,4} the finite conductivity at zero charge-carrier concentration,³ and the strong suppression of weak localization,^{5–8} etc. Most of these properties are direct consequences of the conical dispersion around the Dirac point and the behavior of massless Dirac fermions. Theoretical insights into the exotic transport,^{9,10} the magnetic correlation,¹¹ and the dielectric¹² properties in the graphene systems have also been given. By further confining the electrons in the graphene plane, one can obtain one-dimensional structures which we refer to as graphene nanoribbons (GNRs).¹³ Depending on the cutting direction, GNRs can be either armchair (AGNR) or zigzag (ZGNR) edge. GNRs exhibit physical properties distinct from those of infinite graphene sheets.^{14–19} While the optical response of graphene is in the order of the universal conductance with the absorption around a few per cent in the far infrared and visible range,^{22–25} the response in graphene structures with reduced dimensionality, such as ribbons, can be significantly stronger.^{20,21}

In this paper, we employ a self-consistent approach to reveal some unique electronic properties in ZGNRs subject to a crossed electric and magnetic field. (1) The interplay of the ribbon boundaries and the applied field lead to a very strong electrical polarization along the transverse direction of the ribbon, i.e., the ribbon behaves like a giant electrical dipole. (2) A highly nonlinear Hall current occurs under a moderate electric field of around 5000 V/cm. The ratio of the nonlinear current to the linear current is around 1 at this field strength under a magnetic field of 7.9 T. These properties can only be seen in a self-consistent calculation. Our result shows that a self-consistent approach is very crucial in quantitatively determining the nonlinear effect in graphene nano-

ribbons. The field strength from a non-self-consistent calculation is about 5 times greater in order to achieve the same nonlinear effect.

The problem of charge distribution in GNRs has attracted significant interest recently. With a non-self-consistent approach, energy band structures of GNRs in a perpendicular magnetic field^{26,27} or under a transverse electric field²⁸ have been calculated. The redistribution of charge in GNRs has been investigated using the line charge model,²⁹ however, this breaks down in the vicinity of carbon atoms. Furthermore, it cannot accurately describe on-site energies in the regions near the charge lines. Therefore the non-self-consistent approach used in these works cannot account for any of the new properties demonstrated in this work. Our model combines the self-consistent approach and the discrete nature of the carbon atoms in ZGNRs.

In the tight-binding model and under the nearest neighbor hopping approximation, the Hamiltonian of a GNR in the real space can be written as,

$$H = \sum_i^N \epsilon_i c_i^\dagger c_i + \sum_{\langle i,j \rangle}^N t c_i^\dagger c_j, \quad (1)$$

where ϵ_i denotes the on-site energy which is no longer uniform under an applied electrical field, $\langle i, j \rangle$ denotes the summation of nearest neighbor carbon atoms, and $t \approx 3 \text{ eV}$ denotes the hopping bandwidth. Under a perpendicular magnetic field $\mathbf{B}$, the gauge invariance requires an integral phase to be attached to the hopping energy, $t \rightarrow t \exp[i \frac{2\pi}{\phi_0} \int_i^j \mathbf{A} \cdot d\mathbf{l}]$, where $\phi_0 = ch/e$ is the flux quantum and $\mathbf{A} = (0, Bx, 0)$ is the vector potential for the magnetic field $\mathbf{B} = (0, 0, B)$ in the Landau gauge. We shall use a dimensionless magnetic field strength $f = 3\sqrt{3}Ba^2/2\phi_0$ with $B = |\mathbf{B}|$ and the C-C bond length of graphene $a \approx 1.42 \text{ \AA}$. Here, $f = 1$ corresponds to $B = 7.9 \times 10^4 \text{ T}$. The eigenvalue problem of ZGNR is determined by the Harper equations.^{26,27} From the solutions of the Harper equations together with the potential distribution ϵ_i , we can obtain the energy spectrum and electronic density along the GNR. In the linear response regime, the on-site energy ϵ_i is assumed as $\epsilon_i = Ex_i$, where E is the external

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electric field, and x_i is the site position. However, under a strong electric field, the on-site energy ϵ_i is not only dependent on the external electric field Ex_i but also on the internal potential due to the redistribution of charge in the ribbons. In turn, the internal potential is a function of the applied electric field $U(E)$. In the case of the weak electric field, the effect of the internal potential can be neglected. Under a strong electric field, electron redistribution will take place along the transverse direction of the ribbon. The internal potential caused by the redistribution of charge in the ribbons is determined by Poisson equation $\nabla^2 U(E) = -4\pi\delta\rho(E)$ where $\delta\rho(E) = \rho(E) - \rho(0)$ is the charge density fluctuation induced by the applied electric field. Under a strong field, $\delta\rho(E)$ depends on E nonlinearly and so does $U(E)$. The redistribution of charge and the potential profile can be obtained by solving the Poisson equation self-consistently.

We now use the image charge method and the Green function approach to solve the Poisson equation, i.e., the charge-potential distribution with boundary-value problem exactly (shown in Fig. 1(b)). The on-site electrostatic potential in the discrete site i is written as,

$$\epsilon_i = \frac{1}{4\pi\epsilon} \sum_{i=1}^N \sum_{j=-\infty}^{+\infty} \sum_k \frac{(-)^k q_i}{|\vec{x}_{ijk} - \vec{x}_i|} + Ex_i, \quad (2)$$

where $\epsilon = 5\epsilon_0$ is the graphene permittivity constant, (i, j) denote position coordinate (x, y) , i is chain index, $\vec{x}$ is the lattice point coordinate, x_i is the x coordinate of site with chain index i , q_i denotes the quantities of charge, and k means the number of image charge due to specular reflections. Our approach gives a better microscopic description of the electrostatic potential and charge distribution of GNRs as it takes into account the discreteness of the charge distribution along both the transverse and the longitudinal directions.

The self-consistently determined electron density and potential distribution in a ZGNR of the width $N=20$ are shown in Fig. 2. It is found that free charges in GNRs are forced to the transverse edges by the electric field. This result has important implications when simulating the transport under a strong electric field as the effective electronic screening is modified due to not only the external field but also to the nonlinear charge accumulation edges of GNRs.

FIG. 1. (Color online) (a) A Zigzag graphene nanoribbons, and (b) charge lines and image charges.

For ZGNR, a given chain consists of atoms from the same sublattice and the nearest neighboring chains consist of atoms from the other sublattice. Furthermore, the distance between the nearest neighbor chains is not constant. Therefore, we say that the nearest neighbor chains are inequivalent. As a result, the potential varies from chain to chain in an oscillatory fashion. Here, we should point out that the internal potential is generated by boundary effects and the Lorentz force, not by electron-electron interaction. Because of the inequivalence of the neighboring chains, the charge density also oscillates from one chain to the next (inset of Fig. 2). The most interesting feature of Fig. 2 is the accumulation of opposite charges in the left and right halves of the ribbon. This makes the ribbon behave like a giant electric dipole. Without self-consistency, electrical polarization is much weaker due to the cancellation of opposite charges in the left (or right) half of the ribbon.

Fig. 3(a) shows the energy dispersion and the density of states (DOS) for an $N=20$ ZGNR in the absence of an electromagnetic field. The band structure is gapless at the zone center. The sharp peaks in the DOS correspond to the band inversion points. A perpendicular magnetic field $\mathbf{B} = B\mathbf{e}_z$ or a transverse electric field alone has very little effect on the band structure. Under the perpendicular magnetic field, the Hamiltonian remains invariant under inversion $H(k_y) = H(-k_y)$ and the energy dispersion is symmetric about $k_y = 0$, shown in Fig. 3(b). An E-field along the x -direction does not break the inversion symmetry about the x -axis and the spectrum also remains symmetric about $k_y = 0$, shown in Fig. 3(c). Under crossed E and B fields, the electrons accelerating along the x direction (under E) will gain additional k_y under the B-field. Therefore, the band structure is asymmetric about the $k_y = 0$ as shown in Fig. 3(d). The asymmetry of band structure leads to an asymmetric Hall current distribution in GNRs along the x -axis, giving rise to a non-vanishing total Hall current.

We now calculate the current by integrating over momentum space and summing over all energy bands E_n .

FIG. 2. (Color online) Potential and charge (inset) distribution in a 20-ZGNR. Different curves are for different biases, where ΔU equals to the external electric field strength E times GNR's width.

FIG. 3. The energy band structures and DOS of ZGNR with $N=20$ for (a) $f=0$, $E=0$ V/Å; (b) $f=0.01$, $E=0$ V/Å; (c) $f=0$, $E=0.065$ V/Å; (d) $f=0.01$, $E=0.065$ V/Å.

$$\mathbf{J}_{ij} = \int dk_y \sum_n F(E_n) \left\langle \psi_{jkn} \left| \frac{\partial H}{\partial \mathbf{A}} \right| \psi_{ikn} \right\rangle, \quad (3)$$

$$\mathbf{J}_{total} = \sum \mathbf{J}_{ij}, \quad (4)$$

where $|\psi_{ikn}\rangle$ is the wave function corresponding energy band E_n and $F(E_n)$ is the Fermi distribution function. Fig. 4(a) illuminates that the total current is proportional to the magnetic field for a specific electric field. For the purpose of comparison, we calculate the current without and with a self-consistent potential approach. The x-axis is the electric field strength expressed in terms of total bias across the sample normalized by the hopping energy t . For a 40-unit ZGNR, $x=0.001$ corresponds to a field strength of 7000 V/m. At low voltages, the current is linear in the applied electric field. For a magnetic field of 7.9 T (triangles in Fig. 4(a)), the high order nonlinear transverse current is about the same order of magnitude of the linear current at the field of around 5000 V/cm. In a non-self-consistent approach, the field required to achieve this nonlinear effect is about 5 times greater. The non-self-consistent results are also shown in Fig. 4(a) (dots and diamonds) for comparison.

Under a strong electric field, the current oscillates with voltage. The differential conductance is approximately quantized due to the level quantization. The redistribution of charge in the ribbons happens even without an applied electric field as long as the Fermi energy $E_F > 0$. When $E_F > 0$, there are two types of self-consistent processes in the GNR systems. The first one is that the free charges repel each other. The second one is that the charges are forced to the ribbon edges. As a result, the

corresponding electric potential is higher near the center and lower on the edge. The effect introduced by the bias voltage is insignificant when the external field is infinitesimal and gradually becomes dominant as the field strength increases. Consequently, the self-consistently determined current is weaker under a weak transverse electric field.

The magnetic field strength is given in terms of the dimensionless magnetic flux fraction $f=p/q$. For a fixed value of (q, p) , there exist $2q$ eigen-states in total and each Landau level has a $2p$ -fold degeneracy. For $p=9$ and $q=331$, the distribution of these 662 states is shown in Fig. 4(b). It is shown that the level spacings ΔE_n are approximately proportional to $\sqrt{n}$ in the range of $-1.0t$ to $1.0t$. This implies a characteristic feature of massless Dirac fermions at low energy, as expected for quasi-particles of the honeycomb lattice.^{26,27} Meanwhile, when the energy is above $1.0t$, especially near the top of energy band, the energy spacings approach a constant (as shown in the inset of 4(b)), which is the behavior of normal fermions with parabolic energy-momentum relation. This implies that the properties of charge carriers below and above $1.0t$ are different. Without applied electric field, the Landau levels have $2p$ -fold degeneracy. However, the Landau level degeneracy is lifted when the electric field is applied. From Fig. 4(b), it is found that the electric field lifts the degeneracy of flat Landau levels and makes them dispersive. This behavior originates from the non-uniform potential distribution for cyclotron orbitals centered at different chain locations. The Landau level degeneracy for cyclotron orbitals centered at the same x -position but different y -positions remains.

FIG. 4. (Color online) (a) The total current density of a 40-ZGNR as a function of the transverse electric field under two different magnetic field strengths $B=7.9\text{ T}$ and 15.8 T . The Fermi level is chosen to be $E_F=0.2t$. The x-axis is the field bias across the ribbon in unit of t . SC and NOSC refer to the result calculated self-consistently and non-self-consistently. (b) Formation of Landau levels under a strong magnetic field $f=9/331$. A transverse electric field partly breaks the Landau level degeneracy.

In summary, we have studied the nonlinear electrostatic potential distribution and transport properties of ZGNR under a strong electric field and a perpendicular magnetic field. It is found that ZGNR can be electrically polarized and the nonlinear transverse current response becomes comparable to the linear current at a rather moderate electric field. The field strength required for the nonlinear effect is much weaker from the self-consistent calculation than that from a non-self-consistent calculation.

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- ¹K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, A. A. Firsov, *Science* **306**, 666 (2004).
- ²A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, *Rev. Mod. Phys.* **81**, 109 (2009).
- ³K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, *Nature (London)* **438**, 197 (2005).
- ⁴Y. Zhang, Y. W. Tan, H. L. Stormer, and P. Kim, *Nature (London)* **438**, 201 (2005).
- ⁵H. Suzuura and T. Ando, *Phys. Rev. Lett.* **89**, 266603 (2002).
- ⁶A. F. Morpurgo and F. Guinea, *Phys. Rev. Lett.* **97**, 196804 (2006).
- ⁷D. V. Khveshchenko, *Phys. Rev. Lett.* **97**, 36802 (2006).
- ⁸E. McCann and V. I. Falko, *Phys. Rev. Lett.* **96**, 086805 (2006).
- ⁹H. B. Heersche, P. Jarillo-Herrero, J. B. Oostinga, L. M. K. Vandersypen, and A. F. Morpurgo, *Nature* **446**, 56 (2007).
- ¹⁰M. Müller, J. Schmalian, and L. Fritz, *Phys. Rev. Lett.* **103**, 025301 (2009).
- ¹¹Y. Son, M. L. Cohen, and S. G. Louie, *Nature* **444**, 347 (2006).
- ¹²E. H. Hwang, S. Adam, and S. Das Sarma, *Phys. Rev. Lett.* **98**, 186806 (2007).
- ¹³Y. W. Son, M. L. Cohen, and S. G. Louie, *Phys. Rev. Lett.* **97**, 216806 (2006).
- ¹⁴L. Yang, C. H. Park, Y. W. Son, H. L. Cohen, and S. G. Louie, *Phys. Rev. Lett.* **99**, 186801 (2007).
- ¹⁵L. Brey and H. A. Fertig, *Phys. Rev. B* **73**, 235411 (2006); *Phys. Rev. B* **75**, 125434 (2007).
- ¹⁶H. Zheng, Z. F. Wang, T. Luo, Q. W. Shi, and J. Chen, *Phys. Rev. B* **75**, 165414 (2007).
- ¹⁷Z. F. Wang, Q. W. Shi, Q. Li, X. Wang, and J. G. Hou, *Appl. Phys. Lett.* **91**, 053109 (2007).
- ¹⁸D. Finkenstadt, G. Pennington, and M. J. Mehl, *Phys. Rev. B* **76**, 121405(R) (2007).
- ¹⁹M. Kohmoto and Y. Hasegawa, *Phys. Rev. B* **76**, 205402 (2007).
- ²⁰J. Liu, A. R. Wright, C. Zhang, and Z. Ma, *Appl. Phys. Lett.* **93**, 041102 (2008).
- ²¹A. R. Wright, J. C. Cao, and C. Zhang, *Phys. Rev. Lett.* **103**, 207401 (2009).
- ²²V. P. Gusynin, S. G. Shrapov, and J. P. Carbotte, *Phys. Rev. Lett.* **96**, 56802 (2006).
- ²³A. B. Kuzmenko, E. van Heumen, F. Carbone, and D. van der Marel, *Phys. Rev. Lett.* **100**, 117401 (2008).
- ²⁴R. R. Nair, P. Blake, A. N. Grigorenko, K. S. Novoselov, T. J. Booth, T. Stauber, N. M. R. Peres, and A. K. Geim, *Science* **320**, 1308 (2008).
- ²⁵C. Zhang, L. Chen, and Z. Ma, *Phys. Rev. B* **77**, 241402 (2008).
- ²⁶K. Wakabayashi, M. Fujita, H. Ajiki, and M. Sigrist, *Phys. Rev. B* **59**, 8271 (1999).
- ²⁷J. Liu, Z. Ma, A. R. Wright, and C. Zhang, *J. Appl. Phys.* **103**, 103711 (2008).
- ²⁸V. Lukose, R. Shankar, and G. Baskaran, *Phys. Rev. Lett.* **98**, 116802 (2007).
- ²⁹C. Ritter, S. S. Makler, and A. Latgé, *Phys. Rev. B* **77**, 195443 (2008).