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Liu, Junfeng; Ma, Zhongshui; and Zhang, Chao: Transverse current response in armchair graphene ribbons 2011, 034313-1-034313-5.

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Citation: *J. Appl. Phys.* **110**, 034313 (2011); doi: 10.1063/1.3622323

View online: <http://dx.doi.org/10.1063/1.3622323>

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Transverse current response in armchair graphene ribbons

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(Received 16 June 2011; accepted 2 July 2011; published online 9 August 2011)

We demonstrate that the direction of transverse current in graphene nanoribbons under a magnetic field can be tuned with a gate voltage. It is shown that for armchair ribbons there exist extra energy regions where the direction of the Hall current can be switched between positive and negative values. The directional change of the Hall current coincides with the special points where the two lowest energy bands in the spectrum become degenerate (band crossing points). The number of such degenerate points depends on the width of the ribbons. The dependence of the sign reversal on the gate voltage provides a mechanism for tuning transverse response in graphene based devices. © 2011 American Institute of Physics. [doi:10.1063/1.3622323]

I. INTRODUCTION

Graphene has attracted considerable attention due to its unique electronic properties as well as vast potential applications in nanoelectronic devices.^{1–4} Experimental observations have confirmed the existence of many novel properties, such as electron-hole symmetry, the odd-integer quantum Hall effect,^{2,3} the presence of massless Dirac fermions,⁵ and the minimum conductivity.² Among these, the peculiar odd-integer Hall plateaus have been theoretically recognized in the context of the Landau quantization of massless Dirac fermions.^{6–10} In view of these specific electronic properties, graphene systems with reduced dimensionality such as graphene nanoribbons (GNRs) and graphene fragments (graphene quantum dots) have also become subjects of considerable interest. However, the quantum confinement and edge effects are known to strongly affect the electronic properties of ribbons. These, in turn, modify the physical properties of ribbons and fragments, e.g., unconventional transport and optical excitations.^{11–13} Besides the electronic transport in GNRs with different shapes and widths,^{14–18} the quantum confinement effect on electronic properties of ribbons under a magnetic field has been extensively studied.¹⁹ The quantum confinement effects in GNRs, such as contact resistance, which indirectly relates to the band structure of the ribbons, and the oscillatory behavior of conductivity can play an important role in revealing interesting physics and in developing unique applications.

In this paper, we present a complete evaluation of the transverse conductivity (Hall conductivity) in narrow GNRs subject to a perpendicular magnetic field. The magnetic field causes the electronic motion in the longitudinal direction of the GNRs, shown in Fig. 1. The strength of the magnetic field is sufficiently weak such that the magnetic subband separation is not resolved and band structure is determined by the ribbon confinement. The two most common types of GNR are defined by the shapes of their edges, namely, zigzag edged ribbons (ZGNRs) and armchair edged ribbons (AGNRs). We

show unambiguous evidence for the existence of drastic sign-reversal jumps for the armchair family of GNRs as a function of Fermi energy. While the band-crossings (degenerate points) of ZGNRs occur only at a van Hove singularity, multiple band-crossings are found in the energy spectrum for AGNRs. As a function of Fermi energy, the Hall conductivity undergoes a sign reversal when the energy sweeps over those band-crossings that appear on the band edge. Analyzing corresponding sign reversals in Hall conductivities, we obtain quantum confinement and edge effects on the electronic properties that are distinct from all other properties published so far. We will discuss the evidence for these effects against the intrinsic features emerging from the band structure of an infinite graphene sheet.

The manuscript is organized as follows. In Sec. II we briefly describe the model system. The formalism and calculations of Hall conductivity for zigzag and armchair ribbons are given in Sec. III. In the same section we also analyze the density of states and restoration of van Hove singularity. Concluding remarks are given in Sec. IV.

II. MODELS AND ENERGY BAND STRUCTURE

We describe GNRs by a tight-binding Hamiltonian on a two-dimensional (2D) honeycomb lattice

$$H = t \sum_{\langle ij \rangle} \exp(i\gamma_{ij}) c_i^\dagger c_j,$$

where $\langle i, j \rangle$ denotes the summation over the nearest neighbor sites, t ($= 2.71\text{eV}$) is the hopping integral for nearest neighbors, and $c_i^\dagger$ (c_i) represents the creation (annihilation) operator of electrons on the site i , neglecting the spin degree of freedom. The phase $\gamma_{ij} = (2\pi/\phi_0) \int_i^j A \cdot dl$ is due to the magnetic field applied perpendicularly to the sheet of ribbon, with a vector potential A and the magnetic flux quantum $\phi_0 = hc/e$. The width N of ZGNRs is defined by the number of longitudinal zigzag lines, and by the number of dimer lines for AGNRs. In our calculations, we extend the coupled Harper equations to describe a ribbon of width N with the boundary condition $\psi_0 = \psi_{N+1} = 0$. The corresponding

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FIG. 1. (Color online) An armchair graphene nanoribbon under simultaneous electric and magnetic field. Also shown is the direction of the Hall current.

Hamiltonian can then be written as a $2N \times 2N$ matrix.^{20,21} For a ribbon along the y -direction, the eigenfunctions can be expressed in the form of

$$\psi_{kj} = \zeta_j(k) \exp(iky),$$

where $k = k_y$ is the longitudinal wave vector, j ($j = 1, 2, 3, \dots, 2N$) indicates the channels on the transverse section, and ζ_{kj} denotes the j -th eigenstate which satisfies the equation $H\zeta_{kj} = \epsilon_{kj}\zeta_{kj}$. The energy eigenvalues ϵ_{kj} and the eigenvectors ζ_{kj} can be obtained by a numerical diagonalization of the Hamiltonian. As in any finite system, the energy levels are discrete.

III. HALL CONDUCTIVITY

To calculate the dc Hall conductivity at zero temperature we apply the Kubo formula,²²

$$\sigma_{yx} = -\frac{2\hbar}{W} \sum_k \sum_{\epsilon_{kj}F, \epsilon_{kj'} < E_F} \text{Im} \frac{J_{jj'}^y J_{jj'}^x}{(\epsilon_{kj} - \epsilon_{kj'})^2},$$

where $W = (3N/2 - 1)a$ for ZGNRs and $W = (\sqrt{3}a/2)(N - 1)$ for AGNRs is the width of ribbons with the C-C bond length $a = 0.142\text{nm}$. The current operators J_α ($\alpha = x$ and y) are obtained by

$$J_\alpha = c(\partial H / \partial A_\alpha).$$

In the Hilbert space of eigenvectors ζ_j , the current operators can be represented in terms of a matrix with elements $J_{jj'}^\alpha = \zeta_j^\dagger J_\alpha \zeta_{j'}$, where ζ_j and ϵ_{kj} are the j -th eigenstate and eigenvalue, respectively. As the Fermi energy sweeps through the degenerate point ($\epsilon_{kj} = \epsilon_{kj+1}$) (or band crossing point) the contributions to σ_{yx} from the two crossing subbands become divergent.

A. Hall conductivity of zigzag ribbons

Now we investigate the Hall conductivity for ZGNRs and AGNRs, respectively. In our numerical calculations, the energy is scaled by the hopping integral and the magnetic field is incorporated into the magnetic flux through a plaquette of honeycomb lattice in the unit of a quantum flux, $f \equiv \phi/\phi_0$.

FIG. 2. (Color online) (a) The Hall conductivity vs the Fermi energy for ZGNRs at zero temperature. Widths $N = 10, 20$, and 50 are chosen, with the magnetic flux through a plaquette in the unit of a quantum flux, $f = 1.0 \times 10^{-4}$. (b) The Hall conductivity for $N = 60$ and $f = 2.0 \times 10^{-2}$. (c) The energy spectrum for a ZGNR of width $N = 10$ with $f = 1.0 \times 10^{-4}$ and k_y in the unit of $\pi/\sqrt{3}a$. (d) The evolution of DOS with widening ribbons.

For ZGNRs, the numerical calculations show that band-crossings appear only at $E = \pm|t|$ (Refs. 23 and 24) (Fig. 2(c)). Correspondingly, the Hall conductivity, σ_{yx} , exhibits sign-reversals at $E = \pm|t|$. In Fig. 2(a) we have shown the Hall conductivities for ZGNRs of different widths under the magnetic flux $f = 1.0 \times 10^{-4}$ versus the Fermi energy over the region $0 < E_F < 3|t|$. For $-3|t| < E_F < 0$ the behavior of σ_{yx} is anti-symmetric to that for $0 < E_F < 3|t|$, due to the electron-hole symmetry. Actually, the appearance of jumps at $E = \pm|t|$ is attributed to the van Hove singularity as in infinite graphene sheets.^{26,27} In terms of the energy dispersion, if the main contributions to σ_{yx} are from those processes where both ϵ_{kj} and ϵ_{kj+1} have negative curvature, $\partial^2 \epsilon_{kj} / \partial k^2 < 0$ and $\partial^2 \epsilon_{kj+1} / \partial k^2 < 0$, the Hall conductance σ_{yx} is negative. This is the case for E_F . When $E_F < t$, the situation is the opposite, and σ_{yx} is positive. Increasing the strength of the magnetic field or widening the ribbons leads to the Hall conductivity gradually becoming quantized, as shown in Fig. 2(b). The reason for this is that if the effect of the magnetic field is strong enough, the Landau levels dominate the band structure. Equivalently, when the width of the ribbon is sufficiently increased, the discretization of bands recedes and the Landau levels become dominant. The quantized plateaus in the Hall conductivity are achieved, as has been observed for infinite graphene sheets.

B. Hall conductivity of armchair ribbons

For AGNRs, besides the degenerate point near $E = \pm|t|$ there may emerge some extra band-crossings. The number of crossing points depends on the width of the ribbon. AGNRs can be further divided into two classes, odd and even AGNRs, with widths $N = 2n + 1$ and $N = 2n$, respectively, where n is an integer. Different from only one kind of sublattice at the boundary for ZGNRs, both A and B sublattices

FIG. 3. (Color online) Band structure $E(k)$ for AGNRs with widths $N = 3$ (a), 9(b), 17(c), 21(d), 4(e), 6(f), 14(g) and 18(h), with the magnetic flux $f = 1.0 \times 10^{-4}$ and k_y in the unit of $\pi/3a$. The blue dashed lines and the red circles indicate those crossing points which induce the sign reversals of the Hall conductivities.

occur at the boundary for AGNRs.²⁵ For the odd AGNRs the arrangement of sublattices on the dimer lines of two edges are the same, i.e., A to A and B to B. Thus, there is a reflection symmetry with respect to the middle dimer line of ribbons. However, such a reflection symmetry in the transverse direction is broken in even AGNRs. There is no dimer line in the center of ribbons. The sublattices on the one edge are shifted $3a/2$ along the direction of the ribbons. One distinctive difference between these two-class AGNRs is that there exists a flatband at $E = \pm|t|$ only for odd AGNRs (Figs. 3(a)–(d)), and the flatband is absent for even AGNRs (Figs. 3(e)–(h)). An immediate consequence of this classification is that the density of states at $E = \pm|t|$ is different for the two subclasses of AGNRs. Therefore, the conductivities of the two subclasses would be very different when the Fermi energy sweeps over $E = \pm|t|$. These characteristics imply that there is a further classification index for AGNRs beyond the distinction between metallic ($N = 3m - 1$) and semiconducting ($N \neq 3m - 1$) indices, where m is an integer. In general, the k -independent flat bands at $E = \pm|t|$ become k -dependent in the presence of a magnetic field. Therefore, the Hall conductivities for odd and even AGNRs must be investigated separately.

For odd AGNRs, it is shown in Fig. 4(a) that the flatband provides a sign-reversal jump in Hall conductivity. In addition,

FIG. 4. (Color online) The Hall conductivities at zero temperature vs the Fermi energy for AGNRs of various widths (a) ($N = 3, 9, 17$, and 21) and (b) ($N = 4, 6, 14$, and 18), with the magnetic flux $f = 1.0 \times 10^{-4}$. The evolution of jumps in Hall conductivities for AGNRs with increasing magnetic field strength (c) ($f = 1.0 \times 10^{-4}$, 5.0×10^{-4} , and 1.0×10^{-3} , for a fixed width $N = 21$); and with increasing width (d) ($N = 24, 36$, and 60 , for a fixed magnetic flux $f = 1.0 \times 10^{-4}$). (e) and (f) The DOS for odd and even AGNRs of various widths.

tion, the energy spectrum shows that there exist n subbands above $E = |t|$, and n subbands below $E = |t|$ at $k = 0$ in the region $0 < E < 3|t|$. The two sets of n subbands belong to two different groups, which differ from each other by the shift of $2\pi/3a$ in the k_y dependence. The values of matrix elements $J_{ij}^y J_{jj}^x$ among inter-group bands are small compared to that among the intra-group bands. Thus the degenerate points of the two bands belonging to different groups provide a negligible contribution to the Hall conductivity compared with that from the intra-group degenerate points. There exists a sub-class of degenerate points around which the values of the matrix elements $J_{ij}^y J_{jj}^x$ changes sign when crossing the degenerate point. This sub-class of degenerate points are those at which the two lowest subbands cross each other, $\epsilon_1(k) = \epsilon_2(k)$. We denote these special degenerate points with dashed lines and circles in Figs. 3(a)–3(d). Figure 4(a) shows that the sign-reversal jumps in conductivity occur when the Fermi energy has the values of the energies at these special degenerate points. The anomalous negative σ_{yx} for $E_F < t$ can be further understood from the energy dispersion. At low energies the terms contributing the σ_{yx} are from two neighboring bands of positive curvature, causing σ_{yx} to be positive. Around the first degenerate point, the curvature of $\epsilon_1(k)$ turns negative. Coupled with the diverging energy denominator (which causes the contribution from $\epsilon_1(k)$ and $\epsilon_2(k)$ to denominate), σ_{yx} becomes negative. For these special crossings (circled in red) or special degenerate points, there is changeover from the electron-like to hole-like. For all other

crossings, if the particle is electron (hole)-like before the crossing, it remains electron (hole)-like after the crossing. As E increases further this band ceases to dominate, other bands with positive curvature provide increasingly significant contributions, and σ_{yx} gradually returns to positive. This process will re-occur as the Fermi energy approaches the next special degenerate point.

As the temperature increases, more terms will contribute to σ_{yx} , and the term at the special degenerate point will become less dominant. As a result, the regime of negative σ_{yx} becomes narrower and less drastic, and eventually disappears completely.

The number of special intra-valley degenerate points depends on the width of the ribbons. For those narrow ribbons, the population of subbands is too sparse to form such degenerate points except for the one on the flatband at $E = |t|$. Upon increasing the width of the ribbons, the special degenerate point starts to emerge. The number of such points is fixed for a certain range of ribbon widths, and therefore so too are the number of sign-reversal jumps in Hall conductivity. For example, in the range $N = 3$ to $N = 7$, the special degenerate point occurs only on the flatband. Correspondingly, only one sign-reversal jump appears, at $E_F = |t|$. If the width is increased to $N = 9$, another special degenerate point occurs at $E = 0.52$, and therefore a new sign-reversal jump appears in the Hall conductivity. Furthermore, the second special degenerate point appears only when the ribbon is widened to $N = 15$, and so on.

For even AGNRs, there are also n subbands above $E = |t|$ and n subbands below $E = |t|$ at $k = 0$, as shown in Figs. 3(e)–(h). Figures 3(e)–(h) show the band-crossings below $E = |t|$ for even AGNRs of different widths. It is found that widening the ribbon makes those band-crossings at high energies inhabit states near $E = |t|$, and that they gather exactly at $E = |t|$ in the infinite width limit of a graphene sheet. As discussed above, the special degenerate points give rise to drastic changes in the Hall conductivity. In Fig. 4(b) we have shown the Hall conductivities of even AGNRs for several N . The jumps are attributed to special degenerate points indicated by dashed lines and circles in Figs. 3(e)–3(h). It can be seen that for the narrowest even AGNR, $N = 4$, there are no special degenerate points in the energy spectrum, and therefore no sign reversal jumps in the Hall conductivity. In this width regime the conductivity is also very small. When the ribbon is widened to $N = 6$, the first special degenerate point forms, and a sign reversal jump appears in the Hall conductivity. Widening the ribbons to $N = 12$ and up to $N = 18$, the next special degenerate point appears below $E = |t|$. Correspondingly, the Hall conductivity changes sign. It can be seen that, along with widening ribbons, the last sign reversal jump tends toward $E = |t|$.

It is worth pointing out that, although the ribbons with widths $N = 3m - 1$ (integer m) are metallic, the number of special band crossing points does not change so long as the width lies within a certain range. For example, between $N = 9$ and $N = 15$, AGNRs with width $N = 11$ are metallic, and yet there is still only one special degenerate point below $E = |t|$, similar to the non-metallic cases of $N = 9$, 13, and 15.

C. Density of states and restoration of van Hove singularities

Although the Hall conductivities for ZGNRs and AGNRs of finite widths have been shown to be very different, they reveal the same peculiar odd-integer Hall plateaus for sufficiently wide ribbons. We have seen in Figs. 4(a) and 4(b) that increasing the width lifts the sign-reversal jumps in the low energy region. For sufficiently wide ribbons, the conductivities become positive for $E_F < |t|$, and negative for $E_F > |t|$. The sign change occurs only at $E_F = |t|$. As a demonstration of this, we show the changes caused by increasing the magnetic field in Fig. 4(c) and by varying the ribbon widths in Fig. 4(d). It is well known that both the band structure and density of states (DOS) of a material contain important information about transport properties. Our numerical calculations show that most of the physical features appearing in the DOS of the infinite system could be recovered if the width were increased to $N \simeq 140$ (Figs. 2(d), 4(e), and 4(f)). The whole DOS profile shows that the Dirac fermion and the ordinary fermion are separated at $E = |t|$.^{26,27} For an infinite graphene sheet, the DOS tends to be constant at the Γ point ($E = 3|t|$) due to the parabolic dispersion of ordinary fermions, and vanishes linearly around zero energy due to the relativistic dispersion of Dirac fermions. Further evidence for the effects of edge and quantum confinement can also be identified by comparing our results with the intrinsic band structure of an infinite graphene sheet. As shown in Fig. 2(d), although edge states within the region of $2\pi/3 \leq |k_y| \leq \pi$ (Fig. 2(c)) give rise to a sharp peak in the DOS at zero energy for ZGNRs, it is deduced that as the width of the ribbon increases, the edge states disappear in the limit of a graphene sheet. The absence of the flatband at $E = |t|$ for even AGNRs reflects further evidence of the effects of quantum confinement. This can be examined by the restoration of van Hove singularities in the limit of an infinite graphene sheet. As shown in Fig. 4(f), by increasing the width to a certain region, one can clearly see the emergence of important characteristics of the DOS of an infinite graphene sheet, namely, the buildup of van Hove singularities. Therefore, although the flatband is absent for narrow even AGNRs, it is found that the bands would gather at $E = |t|$ in the infinite width case. The flatband is formed at $E = |t|$, and the DOS becomes a singular at that point. However, the changes of the DOS for $N = 2n + 1$ (Fig. 4(e)) and $N = 2n$ (Fig. 4(f)) in increasing N are not the same. On the one hand, there is the universal feature of the DOS tending to be similar for both odd and even AGNRs. On the other hand, for the region near $E = |t|$, they show very different behaviors when the width of ribbons increases. Although those peaks in the regions near $E = |t|$ are smoothed as the width of AGNRs is increased, the amplitude of the main peak around $E = |t|$ reduces for odd AGNRs, while, on the contrary, a sharp peak at $E = |t|$ emerges for even AGNRs (as shown in the inset of Fig. 4(f)).

IV. CONCLUDING REMARKS

Finally, we comment on the experimental feasibility of our results. The ribbon width of $N = 21$ is now within

fabrication capabilities and has been used in experimental measurements. The best technique used in making sub-10 nm nanoribbon is by cutting the carbon nanotubes,^{28,29} and the smallest carbon nanotube is of $N = 10$.²⁷ The first band-crossing point is not far from the Dirac point. For example, for the ribbon of width $N = 21$, there is one band-crossing at the energy 0.8672 eV and, correspondingly, one jump appears. The density of states around this point is finite and continuous, thus allowing controlled tuning of the Fermi level under gating. The magnetic field intensity for $f = 10^{-4}$ is around 7.9 T, well below the current experimental capability. Therefore, the sign reversal of the Hall effect present here should be experimentally measurable. The result given here is for an intrinsic GNR without the effect of contacts. For a comparison with the experiments, the effect of the contact resistance needs to be subtracted. This procedure is common to electrical measurement of nanometer size systems.

In conclusion, the unusual quantum confinement dependence of sign reversals in the Hall conductivity for narrow ribbons are investigated. It is found that the occurrence of sign-reversal jumps in conductivities is attributed to the band degeneracy of $\epsilon_1(k) = \epsilon_2(k)$. This implies that the total Hall current through the ribbons changes sign as the Fermi energy sweeps over them. We propose that by applying a time-dependent gate voltage oscillating with small amplitude around a given band crossing point, a transverse current oscillation between a positive and negative value can be achieved. This can be the basis for developing another type of graphene based oscillator.

ACKNOWLEDGMENTS

The authors would like to thank Z. B. Li and B. Rosensterin for valuable discussions. This work is supported in part by the National Natural Science Foundation of China No. 10874002 and the Australian Research Council DP0879115.

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