Anisotropic behavior of quantum transport in graphene superlattices:
Coexistence of ballistic conduction with Anderson insulating regime

Jesper Goor Pedersen,1,2 Aron W. Cummings,2 and Stephan Roche2,3

1DTU Nanotech–Department of Micro- and Nanotechnology, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark
2Institut Català de Nanociència i Nanotecnologia (ICN2), Campus de la UAB, Edifici ICN2, 08193 Bellaterra, Barcelona, Spain
3ICREA - Instituto Catalana de Recerca i Estudis Avançats, 08010 Barcelona, Spain

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We report on the possibility to generate highly anisotropic quantum conductivity in disordered graphene-based superlattices. Our quantum simulations, based on an efficient real-space implementation of the Kubo-Greenwood formula, show that in disordered graphene superlattices the strength of multiple scattering phenomena can strongly depend on the transport measurement geometry. This eventually yields the coexistence of a ballistic waveguide and a highly resistive channel (Anderson insulator) in the same two-dimensional platform, evidenced by a $\sigma_{yy}/\sigma_{xx}$ ratio varying over several orders of magnitude, and suggesting the possibility of building graphene electronic circuits based on the unique properties of chiral massless Dirac fermions in graphene.

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Graphene has received significant interest for its unusual transport properties, including phenomena such as Klein tunneling [1] and weak antilocalization [2]. These phenomena preclude the formation of an insulating state at low levels of disorder, in contrast to traditional 2D metallic systems, which are predicted to exhibit insulating states for arbitrarily small disorder strengths [3,4]. This unique behavior makes graphene a promising material for a wide range of next-generation technological applications [5]. One challenging research objective is to maximize the transport anisotropy of graphene, such that it remains a good conductor along one direction while being much more resistive along the other. Such control over the transport properties could be used to direct charge flow and build electronic circuits or waveguides [6], optical circuits [7], or communications devices [8]. For most scattering sources, the transport properties in disordered graphene remain isotropic. More complex forms of disorder, such as structural deformations produced by interaction with a substrate [9,10] or chemical doping [11], produce only moderate transport anisotropies.

A way around this problem involves the creation of graphene superlattices, which are formed from a periodic modulation of the electrical, mechanical, or chemical properties of pristine graphene. It has been theoretically predicted that a strongly anisotropic Fermi velocity can be induced by patterned periodic modifications of the graphene surface [12]. Based on this work, the construction of novel types of graphene electronic devices and circuits from structurally-perfect engineered superlattices was foreseen, attracting significant attention [13–15]. To date however, the inherent disorder introduced through conventional lithography techniques and top-down patterning approaches has impeded the realization of graphene-based superlattices, whose novel transport and device characteristics depend on band-structure engineering, and are thus highly sensitive to disorder [16].

Here, we wish to advocate a different approach to nanostructuring graphene, where instead of considering disorder an inevitable drawback, it serves as beneficial for tuning the properties of graphene. While structural disorder inherent to any fabricated graphene-based superlattice jeopardizes the control of band-structure features, we demonstrate that disorder enables the coexistence of transport regimes which are generally incompatible in conventional conducting materials. Using efficient numerical methodologies, the scaling properties of quantum transport through disordered graphene-based superlattices are demonstrated to become exceedingly anisotropic, resulting in the coexistence of a ballistic transport channel in one direction and a highly resistive channel in the other. We note that similar ideas have been proposed within the field of photonic crystals [17].

We consider a disordered, rectangular lattice of perforations in an otherwise pristine graphene sheet. A given superlattice is referred to via parameters \( \{N_x, N_y\} \), with \( N_y \) denoting the average number of hexagons between the center of the holes along each direction. The lattice constants of the pristine superlattice are \( A_x = \sqrt{3}N_ya \) and \( A_y = N_ya \), respectively, with \( a = 0.246 \) nm the graphene lattice constant. The average size of the antidots is defined via the radius \( R \), which we fix at \( R = 3a \). We consider superlattices for which \( N_x/N_y > 1 \) and refer to the \( y \) and \( x \) directions as the easy and the hard directions, respectively. Disorder is included via parameters \( \delta_x, \delta_y, \delta_R, p_{\text{rem}}, \) and \( N_{\text{rem}} \). Here, \( \delta_x, \delta_y \), and \( \delta_R \) denote the widths of random fluctuations in the centers and radii of holes, respectively. Edge disorder along the holes is added via an iterative process repeated \( N_{\text{rem}} \) times, in which edge atoms are removed with probability \( p_{\text{rem}} \). We remove any dangling bonds in the geometry, i.e., all carbon atoms have at least two nearest neighbors. While structural relaxation is not included, the absence of dangling bonds leads us to expect only a minor influence of potential geometrical relaxation [18]. Throughout this paper we take \( \delta_y = \delta_x = 2a, \delta_R = 0.5a, p_{\text{rem}} = 5\% \), and \( N_{\text{rem}} = 2 \). An example of a disordered [16,9] superlattice is illustrated in Fig. 1. Note that the figure only shows a small, representative domain of the full structure used in the calculations, which contains several millions of atoms. We stress that while we only show results for \( N_x > N_y \), we have confirmed that the results do not depend qualitatively on the orientation of the superlattice with respect to the graphene sheet.

We employ a nearest-neighbor tight-binding model with hopping element \( t = -3 \) eV and set onsite energies to zero. Transport properties are determined numerically via

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an order-$N$ real-space Kubo approach [19–22]. The time- and energy-dependent diffusion coefficient is calculated via $D_\mu(E,t) = \Delta X(E,t)^2/t$, with the mean quadratic displacement $\Delta X(E,t)^2 = Tr[(\delta(E - \hat{H})\hat{X}(t) - \hat{X}(0))^2]/\rho(E)$, where $\rho(E) = Tr[(\delta(E - \hat{H})] \approx$ the density of states. Traces are approximated via initial random phase states and the Lanczos method [23], while the time evolution operator is expanded in Chebyshev polynomials. We use 1500 iterations in the Lanczos method, with broadening included via an imaginary part $\eta = 0.04$ eV of the energy, while the number of Chebyshev polynomials is determined by requiring unitarity of the time evolution operator (within an error of $<10^{-6}$).

The Kubo conductivity, including quantum interference effects, can be calculated from the diffusion coefficients as $\sigma_{xx}(E,t) = e^2 \rho(E) D_x(e,t)/2$, while the semiclassical conductivity reads $\sigma_{xx}^{SC}(E,t) = e^2 \rho(E) \max(D_x(e,t))/2$. Transport properties along the $y$ direction are calculated similarly.

In Fig. 2(a), solid lines illustrate the density of states (DOS) for a pristine [16,9] superlattice. Note the quasi-one-dimensional nature of the DOS with signatures of van Hove singularities, consistent with a picture of the superlattice as an array of weakly coupled nanoribbons aligned along the easy direction. The large aspect ratio of the superlattice unit cell results in a substantial anisotropy of the group velocity $v_y/v_x$, as illustrated in the inset of Fig. 2(a). Note that for larger energies (not shown), such anisotropy is much less pronounced, as expected from the suppression of band structure effects for energies where the electron wavelength becomes much smaller than the hole spacing. While an anisotropic Fermi velocity should affect transport properties, any effect relying critically on periodicity is bound to be quenched significantly in experimental realizations due to the presence of disorder.

We here consider this issue by focusing on lattices displaying significant structural imperfections, inspired by recent experimental fabrications of graphene superlattices [24]. In stark contrast to the pristine case, the DOS of such disordered structures [dashed line in Fig. 2(a)] becomes largely featureless, except for a peak at the Dirac point. The disorder is thus sufficiently strong to wash out the characteristics of the band structure associated with the superlattice. Figure 2(b) shows a zoom of the zero-energy DOS peak. While the DOS resembles that of bulk graphene with short-range impurities [25], the source of the zero-energy peak is different in our case. We attribute the zero-energy peak to states localized predominantly on the hole edges, emerging due to local sublattice imbalances [18,26]. Consistent with this picture, we illustrate in Fig. 2(c) the proportionality of the zero-energy DOS with the density of holes, quantified here via the dimensionless quantity $1/(N_x N_y)$.

As discussed above, the disorder considered is strong enough to quench any effects emerging due to the periodicity of the superlattice (such as anisotropic group velocities). Instead, the scattering sources are determined by the randomness in the positions, radii, and internal geometries of the holes. Despite the largely featureless density of states, this results in drastically different transport properties along the two directions, as illustrated in Fig. 3, showing the diffusion coefficients $D_\mu(E,t)$ for different energies within 1 eV of the Dirac point. Along the easy direction, the time dependence of the diffusion coefficients exhibits (within our accessible timescale of 20 ps) a quasiballistic behavior since $D_y$ does not saturate. In sharp contrast, along the hard axis $D_y(E,t)$ manifests a weak increase at short times before reaching its maximum value and then strongly decays in time, as a result of quantum interferences and localization phenomena [27]. We note that the total elapsed time of 20 ps considered in our calculations corresponds to sample dimensions on the order of 800–1000 nm along the easy direction and 100–180 nm along the hard direction [using $L_\mu(E) = 2\sqrt{t_{\text{max}} D_\mu(E,t_{\text{max}})}$. These results suggest that not only will conductivities along the two directions be of different orders of magnitude, but the temperature dependence should also indicate different transport regimes. In particular, for longer elapsed times (corresponding to wave-packet exploration of larger samples), a metallic behavior for $\sigma_{yy}(T)$ should be measured along one direction, while an insulating behavior for $\sigma_{xx}(T)$ should develop along the other.

In Fig. 3(c) we show the maximum value of the diffusion coefficient within the simulated time span. We attribute the sharp dip near zero energy to the localized zero-energy modes.
Mastodon is a decentralized social networking platform that allows for a more federated and distributed internet. It's designed to be more secure, private, and censorship-resistant. The platform uses a protocol called ActivityPub, which enables users to connect to different instances and interact with each other regardless of where they are hosted. Mastodon supports capabilities such as custom profiles, federated followers, and blocking. It also integrates with other free and open-source software projects, making it a part of a larger ecosystem of software that shares its philosophy and values.

As of today, Mastodon has millions of users worldwide, with a significant number being technology enthusiasts, privacy advocates, and people who value freedom on the internet. The platform continues to evolve and improve, adding new features and capabilities to enhance user experience and security. It remains committed to its mission of providing a more federated and secure social networking experience.
FIG. 5. (Color online) (a) Conductivity vs length for the disorder-
dered superlattice. Red lines show results for the “hard” direction $\sigma_{yy}$, while blue lines indicate results for the “easy” direction $\sigma_{xx}$. Note the logarithmic scale on the ordinate. The horizontal dashed line indicates the minimum value $\sigma_{\text{min}}$ in the absence of quantum interference. (b) Ratio of conductivities calculated at the maximum lengths of the simulated time span of 20 ps. The dashed line indicates the ratio when quantum interference effects are neglected for $\sigma_{\text{xx}}$. Circles indicate the energies corresponding to the results in panel a.

remains metallic and the conductivity remains finite down to zero temperature, whereas the length-dependent decay of $\sigma_{\text{yy}}$ below $\sigma_{\text{min}}$ is evidence of the dominant role played by quantum interferences, which successively drive the electronic state from weak localization to the strong (Anderson) localization regime.

Note that outside the initial transition regime, conductivity along the easy direction becomes more than an order of magnitude larger than along the hard direction within our accessible computational time (or length) scales. This trend is illustrated in Fig. 5(b), where the ratio $\sigma_{yy}(L_{y,\text{max}})/\sigma_{xx}(L_{x,\text{max}})$ is shown. The strongest anisotropy is seen near the Dirac point, where scattering due to edge states around the holes is most pronounced. As we further upscale sample size, the transport anisotropy $\sigma_{yy}(L_y)/\sigma_{xx}(L_x)$ will continuously increase. A crossover to very strong anisotropy will take place once the sample size along the hard direction reaches the directional localization length $\xi_x$. This length scale can be estimated using $\xi_x(E) = l^2(E)\pi h\sigma_{xx}(E)/(2e^2)$ [3]. For the [16,9] superlattice in the absence of long-range impurities, the localization length along the hard direction is of the order of 10 nm, while the localization length along the easy direction is much larger, of order of several thousands of nanometers.

In an experiment, our results suggest that depending on the measurement geometry, the low temperature conductivity could manifest a variable range hopping in the hard direction (similar to the case of damaged graphene [32]) whereas metallic behavior will be measured in the perpendicular direction. To date such strong conductivity anisotropy has never been reported in metallic materials, or disordered graphene. By applying an external magnetic field, one may further tailor the anisotropy in the semiclassical regime [33], while the modulation of magnetotransport features at low fields and the quantum Hall effect at high fields both deserve further consideration.

In conclusion, we have shown that disorder, while destroying anisotropic velocity renormalization in perfect graphene superlattices, can result in large anisotropic conductivities by inducing strong localization along the hard direction of transport. These results suggest that disorder could serve as an inherent tool in the field of nanostructured graphene, giving rise to different transport properties of massless Dirac fermions.

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