



Signatures of Klein tunneling in disordered graphene p - n - p junctions

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We present a method for obtaining quantum transport properties in graphene that uniquely combines three crucial features: microscopic treatment of charge disorder, fully quantum-mechanical analysis of transport, and the ability to model experimentally relevant system sizes. As a pertinent application we study the disorder dependence of Klein tunneling dominated transport in p - n - p junctions. Both the resistance and the Fano factor show broad resonance peaks due to the presence of quasi-bound-states. This feature is washed out by the disorder when the mean free path becomes of the order of the distance between the two p - n interfaces.

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A realistic modeling of quantum transport in graphene¹ has two main requirements: microscopic treatment of disorder and a fully quantum-mechanical calculation of transport, taking into account the finite (but large with respect to the lattice constant) size of the samples. This is especially important close to the Dirac point,² the charge neutrality point at which transport is dominated by evanescent modes and conventional analytical methods fail, and for interference effects. In this Rapid Communication we report on such a calculation in a study of the resistance oscillations in a disordered graphene p - n - p junction which incorporates both realistic Coulomb disorder and quantum-mechanical transport.

The physics of the p - n - p junction is governed by “Klein tunneling,” an effect first discovered in the context of a relativistic particle tunneling through a potential barrier with a height comparable to its rest energy.³ Since the occurrence of relativistic Klein tunneling is a crucial feature distinguishing graphene from ordinary electronic materials, a clear understanding of how to unambiguously observe Klein tunneling in realistic graphene samples, where disorder is unavoidably present, is important. In graphene, transmission through a potential barrier has a pronounced angular dependence, with perfect transmission for perpendicular incidence and a quick decrease of transmission probability for finite angle of incidence.⁴ As a consequence, electrons can be confined within a single potential barrier, such as the p - n - p junction.^{5,6} Resonant tunneling through those confined states then leads to pronounced oscillations in the resistance as a function of system parameters.⁵⁻⁷

The existence of this phenomenon relies heavily on the presence of a well defined interface between the p and n regions. Long-range disorder induces the formation of electron-hole puddles⁸⁻¹¹ which make the study of Klein tunneling effects in disordered p - n - p junctions highly nontrivial. Early experiments failed to reproduce the predicted resistance oscillations,^{12,13} presumably because of too much disorder.¹⁴ More recent experiments that seek to minimize the effects of disorder have been more successful.^{15,16} However a theoretical understanding of whether or to what extent these experiments are really observing Klein tunneling phe-

nomena and the issue of the experimental conditions needed to see Klein tunneling unambiguously have remained open.

There exists strong evidence that disorder in current experiments is dominated by remote charged impurities^{17,18} invariably present in the graphene environment. Due to the long-range character of the Coulomb potential of impurity and gate charges, all scattering potentials and charge densities in the graphene sheet vary slowly on the scale of the lattice constant. This fact leads to two simplifications that make an accurate modeling of current experimental setups^{13,15,16} possible. First, the Thomas-Fermi-Dirac (TFD) self-consistent density-functional method is sufficient to obtain the ground-state carrier density in the presence of disorder.^{10,19} Second, intervalley coupling can be neglected for a smooth scattering potential so that one can model transport using the single valley Dirac Hamiltonian. The transfer-matrix method of Refs. 20 and 21 is ideal for this purpose and can be used for experimentally relevant system sizes, as opposed to tight-binding models which are generally limited to small system sizes.

Our calculation thus consists of two steps. In the first step the ground-state carrier density $n(\mathbf{r})$ and the corresponding screened Coulomb potential V_{sc} is obtained using the TFD approach.¹⁰ In the second step the resistance and Fano factor, the ratio of shot noise power and electrical current, are calculated using V_{sc} as an input into the fully quantum-mechanical transfer-matrix approach.^{20,21} We first describe the two steps of our method in more detail and then turn to the results.

A schematic of the p - n - p junction under consideration is shown in Fig. 1(a). A top gate of length L_{tg} is located a distance d_{tg} above the graphene layer—in an air-bridge setup the medium in between is air with dielectric constant $\epsilon_1=1$. A back gate that controls the average carrier density is separated from the graphene by a SiO₂ substrate (dielectric constant $\epsilon_2=4$). The effective dielectric constant in this setup is $\epsilon=(\epsilon_1+\epsilon_2)/2$. Together, the voltages on these two gates define the junction. Examples of potential profiles are shown in Fig. 1(b).

A number of charged impurities are trapped in the substrate and just below the graphene layer. We model this by a

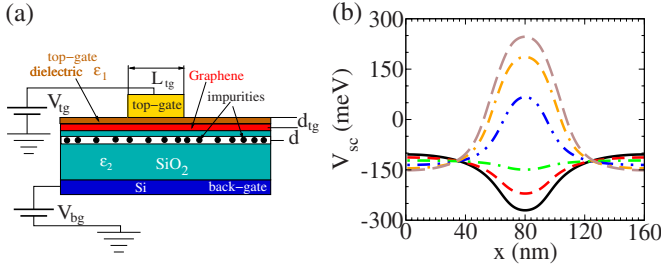


FIG. 1. (Color online) (a) A schematic of the top gated setup. Graphene is represented by the red layer and the top-gate dielectric by a brown one. (b) Profile of the screened potential V_{sc} in the absence of disorder. The back gate density is fixed at $n_{bg}=5 \times 10^{11} \text{ cm}^{-2}$ and (from bottom to top) $\Delta n_{tg}=-5 \times 10^{12} \text{ cm}^{-2}$ to $5 \times 10^{12} \text{ cm}^{-2}$ in steps of $2 \times 10^{12} \text{ cm}^{-2}$. All results in this Rapid Communication were obtained for square samples of size $W=L=160 \text{ nm}$ assuming $L_{tg}=30 \text{ nm}$, $d_{tg}=10 \text{ nm}$, $d=1 \text{ nm}$, $\epsilon_1=1$ (air), and $\epsilon_2=4$ (SiO_2).

random distribution $C(\mathbf{r})$ of impurity charges at a fixed distance d with properties

$$\langle C(\mathbf{r}) \rangle = 0; \quad \langle C(\mathbf{r}_1)C(\mathbf{r}_2) \rangle = n_{\text{imp}}\delta(\mathbf{r}_2 - \mathbf{r}_1), \quad (1)$$

with n_{imp} the average 2D charge impurity density.

In the TFD approximation, the ground-state carrier density $n(\mathbf{r})$ in the graphene layer is obtained by minimizing the energy functional

$$E[n] = \int d^2\mathbf{r} n(\mathbf{r}) \left[\frac{2}{3} \hbar v_F |\pi n(\mathbf{r})|^{1/2} + V_{sc}(\mathbf{r}) \right] + E_{xc}[n] \quad (2)$$

with respect to $n(\mathbf{r})$. Here $v_F \approx 10^6 \text{ m/s}$ is the Fermi velocity for graphene,

$$V_{sc}(\mathbf{r}) = \hbar v_F r_s \left[V_d(\mathbf{r}) + V_{tg}(\mathbf{r}) + \frac{1}{2} \int d^2\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \right] - \hbar v_F \mu, \quad (3)$$

with $r_s \equiv e^2 / \hbar v_F \epsilon$, V_d and V_{tg} the potentials induced by the impurity density $C(\mathbf{r})$ and the top gate, respectively, and μ the chemical potential. $E_{xc}[n]$ is the exchange-correlation energy (see Refs. 10 and 22 for details) which we include even though it gives only minor quantitative corrections to the transport properties of the p - n - p junction. The minimization is subject to the constraint $(1/A') \int_A n(\mathbf{r}) d^2r = n_{bg}$, where A' is the area of the sample where the top-gate potential is negligible (in practice we obtain accurate results by excluding the area directly below the top gate plus a 10 nm wide buffer region on each side). The constraint is enforced self-consistently by varying μ . The electrostatic potential V_{tg} is expressed in terms of the top-gate charge density n_{tg} ,

$$V_{tg}(\mathbf{r}) = \int d^2\mathbf{r}' \frac{n_{tg}(\mathbf{r}')}{(|\mathbf{r} - \mathbf{r}'|^2 + d_{tg}^2)^{1/2}}, \quad (4)$$

and is obtained self-consistently, for a fixed voltage difference between the top gate and graphene, φ_{tg} , by requiring that in the region below the top gate

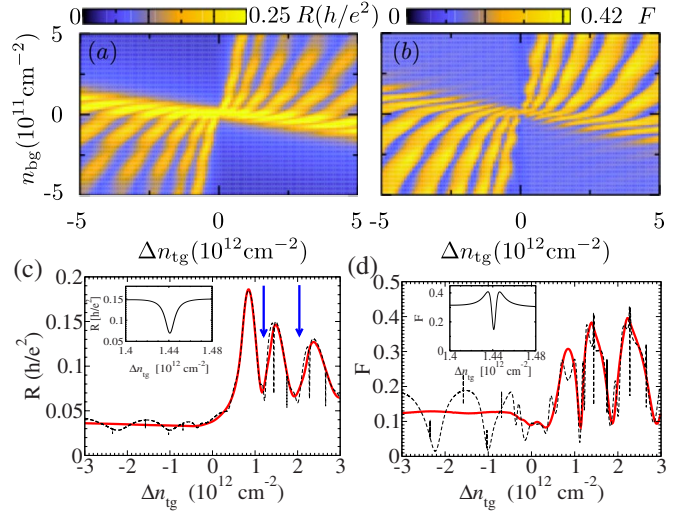


FIG. 2. (Color online) Gate voltage dependence of (a) resistance and (b) Fano factor of a clean device. A single trace of (c) resistance and (d) Fano factor at a fixed back gate density $n_{bg}=5 \times 10^{11} \text{ cm}^{-2}$. The smooth curves are obtained by averaging over boundary conditions. The arrows in (c) indicate the positions of the resistance minima obtained using Eq. (7). The insets show a close up of one of the narrow resonances obtained for transverse periodic boundary condition.

$$\Delta n_{tg} \equiv n_{tg}(\mathbf{r}) - n(\mathbf{r}) = C_{tg} \varphi_{tg} / |e|,$$

where C_{tg} is the top-gate capacitance.

The potential V_{sc} defines a scattering problem through the Dirac Hamiltonian

$$H = v_F \mathbf{p} \cdot \boldsymbol{\sigma} + V_{sc}(\mathbf{r}) \quad (5)$$

with $\sigma = (\sigma_x, \sigma_y)$ the Pauli matrices. The Schrödinger equation $H\psi=0$ generates a transfer matrix \mathcal{M} , which relates the wave function at $x=0$ to the one at $x=L$, $\psi_L = \mathcal{M}\psi_0$. In order to numerically calculate \mathcal{M} we divide the interval $(0, L)$ into N equal subintervals of length $\delta x = L/N$ and calculate the transfer matrix in each subinterval in the Born approximation. This gives²¹

$$\mathcal{M} = \prod_{n=1}^N e^{-i/2 \delta x \partial_y \sigma_z} e^{-i u_n \sigma_x} e^{-i/2 \delta x \partial_y \sigma_z}, \quad (6a)$$

$$u_n(y) = \frac{1}{\hbar v_F} \int_{(n-1)\delta x}^{n\delta x} dx V_{sc}(x, y). \quad (6b)$$

We then take the limit $N \rightarrow \infty$ in which the Born approximation becomes exact. From the transfer matrix \mathcal{M} we calculate the matrix t of transmission amplitudes, which in turn gives us the two terminal conductance and Fano factor as $G = R^{-1} = (4e^2/h) \text{tr} t t^\dagger$ and $F = \text{tr}[(1 - t t^\dagger) t t^\dagger] / \text{tr} t t^\dagger$.

We now turn to our results. We first consider the clean case $n_{\text{imp}}=0$. By varying the top-gate potential, the junction type can be varied from p - n - p to p - p - p (or n - p - n to n - n - n depending on the back gate voltage), as shown in Fig. 1(b). The dependence of the resistance R and Fano factor F on the two gate voltages is shown in Figs. 2(a) and 2(b). In the

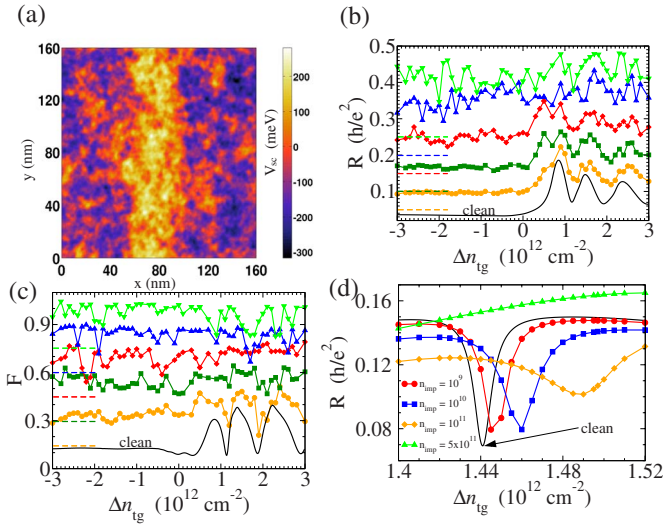


FIG. 3. (Color online) (a) $V_{sc}(\mathbf{r})$ for a disordered junction with $n_{bg}=5 \times 10^{11} \text{ cm}^{-2}$, $\Delta n_{tg}=2 \times 10^{12} \text{ cm}^{-2}$, and $n_{imp}=5 \times 10^{11} \text{ cm}^{-2}$. (b) Resistance and (c) Fano factor in the presence of disorder (single realization) for a fixed back gate density $n_{bg}=5 \times 10^{11} \text{ cm}^{-2}$ and several values of the impurity density (from bottom to top $n_{imp}=0, 1, 2.5, 5, 10$, and $15 \times 10^{11} \text{ cm}^{-2}$). The disordered curves have been shifted for clarity, with dashed lines showing their zero. (d) The top-gate density dependence of the resistance at a narrow resonance for different values of the impurity density.

p - p - p (n - n - n) region of the upper left (lower right) corner the resistance is small compared to the resistance of the p - n - p (n - p - n) region of the upper right (lower left) corner. Pronounced oscillations in the resistance are seen in the p - n - p and n - p - n regions. The behavior of the Fano factor mostly follows that of the resistance.

The resistance oscillations can be understood as arising from resonances through quasi-bound-states inside the barrier created by the two p - n interfaces.⁵⁻⁷ The larger the transverse momentum q_y , the larger the incident angle for scattering off the barrier and the tunneling amplitude decreases. The broad oscillations arise from resonant tunneling of the few modes with smallest q_y . Larger q_y give rise to very narrow resonance seen in Figs. 2(c) and 2(d), where we show a cross section of Figs. 2(a) and 2(b) at a fixed value of the back gate voltage in a higher resolution. Since the positions and widths of the narrow resonances are sensitive to the transverse boundary conditions we also plot the smooth curves obtained by averaging over twisted boundary conditions. The weak oscillations in the p - p - p and n - n - n regions and the narrow resonances are absent after the averaging. Observation of the narrow resonances will thus require very well defined edges.

In contrast to the narrow resonances the resistance minima for the broader oscillations do not depend on boundary conditions and can be estimated by a semiclassical argument.⁵ One can think of the p - n - p junction as a Fabry-Perot etalon in which waves scattered off the two p - n interfaces interfere destructively if the WKB phase

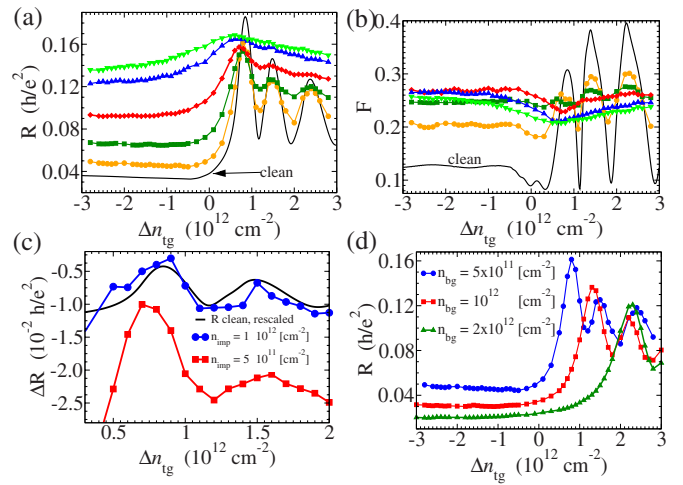


FIG. 4. (Color online) Disorder averaged resistance (a) and Fano factor (b) as a function of Δn_{tg} for different values of n_{imp} [parameters and color coding the same as in Fig. 3(b)]. (c) The resistance difference ΔR where we have subtracted the resistance at $n_{imp}=1.5 \times 10^{12} \text{ cm}^{-2}$ where the transport is diffusive, to emphasize the survival of broad oscillations for n_{imp} as high as 10^{12} cm^{-2} . (d) Disorder averaged R as a function of Δn_{tg} for different values of n_{bg} .

$$\theta_{\text{WKB}} = - \int_{x_1}^{x_2} V_{sc}(x', y) dx' \equiv 0 \pmod{\pi}, \quad (7)$$

with the turning points x_i defined by the condition $V_{sc}(x_i, y) = 0$, $i=1, 2$. The positions of the resistance minima that follow from this argument are indicated by arrows in Fig. 2.

We now consider the effect of disorder. A single realization of the scattering potential V_{sc} in a disordered p - n - p junction is shown in Fig. 3(a). For realistic impurity concentrations, the correlation length of V_{sc} is $\sim 10 \text{ nm}$.^{10,11} While one can still clearly make out the different p and n regions in the presence of disorder, the boundary between the two is no longer as sharp, leading to a weaker confinement of particles inside the barrier. The effects of Klein tunneling are thus expected to be suppressed.

Figures 3(b) and 3(c) give the transport properties as a function of top-gate voltage for a single disorder realization and for different impurity densities. Mesoscopic fluctuations due to the disorder are superimposed on the oscillations from the Klein tunneling. As the impurity strength increases these fluctuations become stronger, eventually dominating the signal. The Fano factor is more sensitive to disorder than the resistance. The effect of disorder on a narrow resonance is shown in Fig. 3(d).

In Fig. 4 we show the disorder averaged resistance and Fano factor, where the average was taken over 10^3 disorder realizations. We find that the clean limit broad quantum oscillations survive for impurity densities up to $n_{imp} \sim 10^{12} \text{ cm}^{-2}$ while the narrow resonances disappear at $n_{imp} \sim 10^{11} \text{ cm}^{-2}$. We do emphasize that for weak enough disorder and well defined edges the narrow resonances will be present, and it is therefore conceivable that they may actually be observed at low enough temperatures.

As in the case of the single disorder realization, the dependence of the Fano factor on the disorder strength is similar to that of the resistance. The dependence of the resistance on the back gate voltage for a fixed impurity density is shown in Fig. 4(d). The main effect of the back gate is an overall reduction of the resistance and a shift of the top-gate density at which the central region changes polarity.

One expects impurity scattering effects to start dominating the ballistic oscillations when the mean free path l becomes comparable to the sample width W (for the narrow resonances) or the length of the central n region (for the broad oscillations). The mean free path l can be estimated through its relation to the conductivity σ , $l=(h/2e^2)(\sigma/k_F)$, where k_F is the Fermi wave vector. Away from the Dirac point, $\sigma=(2e^2/h)\langle n\rangle/n_{\text{imp}}f(r_s,d)$,²³ where $f(r_s,d)$ is a known function of r_s and d only [$f(r_s=0.8, d=1\text{ nm})=0.1$].²⁴ Setting $\langle n\rangle=n_{\text{bg}}$ and using the impurity densities quoted above, we find that the narrow resonances vanish for $l\approx 400$ nm, which is the same order of magnitude as expected. The impurity density at which the broad oscillations disappear corresponds to a mean free path $l\approx 40$ nm. This is roughly the same as the length, L_{pn} , between the two p - n interfaces, see Fig. 1, and consistent with the experimental results of Refs. 15 and 16. Note that since L_{pn} increases with Δn_{tg} [cf. Fig. 1(b)] the resistance peaks at high Δn_{tg} are more sensitive to disorder.

Finally we comment on the effects of the dielectric envi-

ronment. Changing $\epsilon\propto 1/r_s$ is not expected to have any qualitative effects. Through the r_s dependence of the mean free path, the impurity density at which the Klein tunneling remains observable scales as $1/f(r_s,d)$ which increases with ϵ . Further, since the scattering potential V_{sc} is proportional to r_s the distance in Δn_{tg} between the resistance maxima scales roughly as $1/r_s$.

In summary, we have presented a powerful theoretical method that is generally applicable to transport problems in realistic graphene samples where the disorder is dominated by charge impurities and transport properties need to be obtained fully quantum mechanically. In particular we have applied the method to understand the effects of disorder on transport through p - n - p junctions. The crossover from the ballistic transport governed by Klein tunneling, to the disordered diffusive transport is found to take place as the mean free path becomes of the order of the distance between the two p - n interfaces consistent with recent experiments.^{13,15}

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- ¹K. S. Novoselov *et al.*, *Science* **306**, 666 (2004).
²A. H. Castro Neto *et al.*, *Rev. Mod. Phys.* **81**, 109 (2009).
³N. Dombey and A. Calogeracos, *Phys. Rep.* **315**, 41 (1999).
⁴T. Ando, T. Nakanishi, and R. Saito, *J. Phys. Soc. Jpn.* **67**, 2857 (1998); M. I. Katsnelson, K. S. Novoselov, and A. K. Geim, *Nat. Phys.* **2**, 620 (2006); V. V. Cheianov and V. Fal'ko, *Phys. Rev. B* **74**, 041403(R) (2006).
⁵P. G. Silvestrov and K. B. Efetov, *Phys. Rev. Lett.* **98**, 016802 (2007).
⁶J. H. Bardarson, M. Titov, and P. W. Brouwer, *Phys. Rev. Lett.* **102**, 226803 (2009).
⁷A. V. Shytov, M. S. Rudner, and L. S. Levitov, *Phys. Rev. Lett.* **101**, 156804 (2008).
⁸E. H. Hwang, S. Adam, and S. Das Sarma, *Phys. Rev. Lett.* **98**, 186806 (2007).
⁹J. Martin *et al.*, *Nat. Phys.* **4**, 144 (2008).
¹⁰E. Rossi and S. Das Sarma, *Phys. Rev. Lett.* **101**, 166803 (2008).
¹¹Y. Zhang *et al.*, *Nat. Phys.* **5**, 722 (2009).
¹²B. Huard, J. A. Sulpizio, N. Stander, K. Todd, B. Yang, and D. Goldhaber-Gordon, *Phys. Rev. Lett.* **98**, 236803 (2007); J. R. Williams, L. DiCarlo, and C. M. Marcus, *Science* **317**, 638 (2007); B. Özyilmaz, P. Jarillo-Herrero, D. Efetov, D. A. Abanin, L. S. Levitov, and P. Kim, *Phys. Rev. Lett.* **99**, 166804 (2007).
¹³N. Stander, B. Huard, and D. Goldhaber-Gordon, *Phys. Rev. Lett.* **102**, 026807 (2009).
¹⁴M. M. Fogler, D. S. Novikov, L. I. Glazman, and B. I. Shklovskii, *Phys. Rev. B* **77**, 075420 (2008).
¹⁵R. V. Gorbachev *et al.*, *Nano Lett.* **8**, 1995 (2008).
¹⁶A. F. Young and P. Kim, *Nat. Phys.* **5**, 222 (2009).
¹⁷Y.-W. Tan, Y. Zhang, K. Bolotin, Y. Zhao, S. Adam, E. H. Hwang, S. Das Sarma, H. L. Stormer, and P. Kim, *Phys. Rev. Lett.* **99**, 246803 (2007).
¹⁸J. H. Chen *et al.*, *Nat. Phys.* **4**, 377 (2008).
¹⁹E. Rossi, S. Adam, and S. Das Sarma, *Phys. Rev. B* **79**, 245423 (2009).
²⁰M. Titov, *Europhys. Lett.* **79**, 17004 (2007).
²¹J. H. Bardarson, J. Tworzydło, P. W. Brouwer, and C. W. J. Beenakker, *Phys. Rev. Lett.* **99**, 106801 (2007).
²²M. Polini, A. Tomadin, R. Asgari, and A. H. MacDonald, *Phys. Rev. B* **78**, 115426 (2008).
²³K. Nomura and A. H. MacDonald, *Phys. Rev. Lett.* **96**, 256602 (2006); T. Ando, *J. Phys. Soc. Jpn.* **75**, 074716 (2006); V. V. Cheianov and V. I. Fal'ko, *Phys. Rev. Lett.* **97**, 226801 (2006).
²⁴S. Adam *et al.*, *Proc. Natl. Acad. Sci. U.S.A.* **104**, 18392 (2007).