Veselago lens and Klein collimator in disordered graphene

To cite this article: F Libisch et al 2017 J. Phys.: Condens. Matter 29 114002

View the article online for updates and enhancements.

Related content
- Focusing RKKY interaction by graphene P–N junction
  Shu-Hui Zhang, Jia-Ji Zhu, Wen Yang et al.
- Coherent transport through graphene nanoribbons in the presence of edge disorder
  F Libisch, S Rotter and J Burgdörfer
- Transport through graphene quantum dots
  J Güttinger, F Molitor, C Stampfer et al.
Veselago lens and Klein collimator in disordered graphene

F Libisch¹, T Hisch, R Glattauer, L A Chizhova and J Burgdörfer

Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10/136, A-1040 Vienna, EU, Austria

E-mail: florian@concord.itp.tuwien.ac.at

Received 2 September 2016, revised 20 December 2016
Accepted for publication 3 January 2017
Published 7 February 2017

Abstract

We simulate electron transport through graphene nanoribbons of realistic size containing a p–n junction patterned by electrostatic gates. For a sharp p–n interface, Klein tunneling leads to refocusing of a divergent beam forming a Veselago lens. Wider transition regions allow only electrons with near-perpendicular incidence to pass the junction, forming a Klein collimator. Using a third nearest neighbor tight binding description we explore the influence of interface roughness and bulk disorder on guiding properties. We provide bounds on disorder amplitudes and p–n junction properties to be satisfied in order to experimentally observe the focusing effect and compare our predictions to very recent realizations.

Keywords: graphene, nanoelectronics, Klein tunneling, Veselago lens

(Some figures may appear in colour only in the online journal)
collimators are robust in the presence of moderate interface roughness and weak bulk disorder, and give quantitative constraints for experimental realizations.

2. Klein tunneling

The linear band crossing in graphene at the $K$-point, the so-called Dirac point creates a double-cone structure that closely mimics the dispersion relation of massless Dirac fermions (see figure 1(a)), described by the Dirac-like Hamiltonian,

$$H = v_F \begin{pmatrix} 0 & p_x + i p_y \\ p_x - i p_y & 0 \end{pmatrix} + \mathbb{1} \cdot V(x),$$

(1)

where $p_x$ ($p_y$) denote the momentum operators and we have set $E(k_F) = 0$. The approximation (1) ignores both the length scale of the graphene lattice constant $a = 1.4$ Å and the broken rotational symmetry of the cone due to the hexagonal lattice structure, an effect known as trigonal warping [8]. The symmetric electron-like (hole-like) dispersion relation of equation (1) above (below) the Dirac point allows to locally tune the Fermi energy to create n-doped (electron-like) or p-doped (hole-like) regions of carrier density by an external potential. At a finite-width potential step $V(x)$ (by, e.g. a back gate) [8] (see figure 1)

$$V(x) = \begin{cases} V_0 \cdot x/d & |x| < d \\ \text{sgn}(x) \cdot V_0 & |x| \geq d \end{cases}$$

(2)

between an n-doped and a p-doped region, electrons may tunnel from the n-region into the p-region (see figure 1). In the limit of a sharp interface with the transition half-width $d$ small compared to the de Broglie wavelength $\lambda_D$, $d \ll \lambda_D$, tunneling occurs with near unit probability due to the electron-hole symmetry of $H$ (equation (1)), a phenomenon known as Klein tunneling [15, 32]. Since the group velocity is reversed when switching from the upper to the lower cone, i.e. from the n to the p region, the wave originally propagating in the $(k_x, k_y)$ direction in the n-region is transmitted into the p region with wavevector $(-1) \cdot (-k_x, k_y) = (k_x, -k_y)$ due to flux conservation at the interface. The resulting scattering kinematics corresponds to the optical analogue of a metamaterial with a negative index of refraction (figure 1). Consequently, a diverging ray of trajectories emanating from a source point (5) will be focused by an ideal p–n interface onto the point $F$. Such an electron-optical lens could be created in graphene simply by applying a discontinuous potential step. If, however, the transition from n- to p- region is gradual instead of sudden, i.e. if $d$ is of the order of $\lambda_D$, new effects appear. For grazing incidence with $|k_x| \gg |k_y|$ at the p–n interface, $k_y$ may exceed the local $k(x) = |E_F - V(x)|/\hbar v_F$ causing total reflection rather than transmission. Consequently, partial transmission through the p–n interface is restricted to near-normal incidence [28] and no distinct focal point exists. The p–n junction operates in this regime as filter that only transmits on near-normal incidence.

3. p–n junction in graphene nanoribbons

Realizing electron-optical elements such as lenses and filters suggested by the ideal massless Dirac fermion picture (equation (1)) in graphene structures must account for the discrete honeycomb lattice structure with lattice constant $a$ made up by two interleaved triangular sublattices (A and B). It can be described in tight-binding approximation by the Hamiltonian [33]

$$H = \sum_i \langle \phi_i | V(x) | \phi_i \rangle - \sum_{(i,j)} \gamma_{ij} \langle \phi_i | \phi_j \rangle + \text{h.c.},$$

(3)

where the sum $(i,j)$ extends over pairs of lattice sites, $\phi_i$ is the tight-binding orbital with spin $s$ at lattice site $j$, $V$ is a locally varying potential which includes in the present case the potential step (equation (2)), and $\gamma_{ij}$ are the hopping matrix elements between lattice sites $i$ and $j$. We omit physical spin in the following. In contrast to the Dirac Hamiltonian of equation (1), the electronic structure of graphene features a weakly broken electron-hole symmetry accounted for in the present simulations by including third-nearest-neighbor coupling (for details see [34]). Furthermore, the hexagonal symmetry of the graphene lattice distorts the perfectly circular Dirac cone at energies farther away from the Dirac point. This so-called trigonal warping [8, 37] is also included in our third-nearest-neighbor description.

We explore the consequences of this symmetry breaking for a graphene nanoribbon that extends to infinity to the left and right, $(x \to \pm \infty)$, containing a single p–n transition.

Figure 1. (a) Graphene bandstructure near a p–n junction with transition width $2d$. Circles represent cuts through the Dirac cone at constant energy, the arrow gives the direction of group velocity. (b) Refraction at an ideal infinitely sharp p–n junction with zero transition width $d = 0$ results in focusing due to the different sign of the group velocity for the particle and hole. (c) Same as (b) for a finite transition width between n- and p-region, leading to specular reflection of rays incident with large perpendicular momentum component $d$ results in focusing due to the different sign of the group velocity for the particle and hole.
Note that a flake of finite size would be unsuitable to realize focusing of rays as bound state effects of the finite-size flake would overshadow the propagation. We therefore use open boundary conditions within the framework of an effective Hamiltonian

\[ H_{\text{eff}} = H + \Sigma_L(E) + \Sigma_R(E), \]

where the energy-dependent self-energy matrices \( \Sigma_L(E) \) and \( \Sigma_R(E) \) describe the coupling to half-infinite waveguides to the left (L) and right (R) via \( \Sigma_L = H_L G_L H^\dagger \), \( \Sigma_R = H_R G_R H^\dagger \). Here, \( G_L \) and \( G_R \) represent the surface Green’s functions of the perfect half-infinite waveguides, and \( H \) the interaction Hamiltonian between the leads and the simulated structure. \( H_n \), and consequently the self-energy corrections \( \Sigma_L, \Sigma_R \) are non-zero only on to the outermost carbon atoms to the left and right. Note that \( H_{\text{eff}} \) is no longer Hermitian since the open boundary conditions introduce a finite lifetime of states.

The width \( W \) of the nanoribbon plays a key role for observing lens or collimator effects. Only for sufficiently large width \( W \gg \lambda_0 \) (for more quantitative estimates see below) pronounced lens effects appear while for smaller \( W \) distortions by reflection at the boundary largely mask the effects. The simulation of such wide ribbons (1200 lattice sites in transverse direction for \( W = 300 \text{ nm} \)) represents a numerical challenge. The simulation of such wide ribbons (1200 lattice sites in transverse direction for \( W = 120 \text{ nm} \)) includes several million carbon orbitals. We consider a point source \( (S) \) on the n side \((S) = W = 120 \text{ nm} \) a potential step of width \( W \). For a doping of \( E = V_0 = 0.5 \text{ eV} \) corresponding to a p–n step height of \( 2V_0 = 1 \text{ eV} \), \( \lambda_0 \) follows from the relation

\[ \lambda_0 E = h v_F \approx 3.5 \cdot \text{nm eV}, \]

as \( \lambda_0 \approx 7 \text{ nm} \). Choosing the distance of \( S \) from the interface \( |x_S| = 25 \text{ nm} \), we have \( |x_S|/\lambda_0 \gg 3.5 \) for which pronounced focusing effects are already expected. In order to prevent the reduction of the visibility of focusing by boundary reflections, \( W \) should be large compared to \( |x_S| \). Combining these two constraints implies \( W \gg \lambda_0 \) indicating that only in wide p–n junctions Veselago lens and Klein collimation are clearly visible. We observe focusing of the ray down to the diffraction limit with the lateral width \( s \) of the focal spot at \( F \) close to \( 2s \approx \lambda_0 \). We have, furthermore, numerically verified that distributing the source point over a small area \( S \) of size \( \lambda_0^2 \) does not significantly change the focusing pattern. Likewise, a finite energy resolution \( \Delta E \), as long as \( \Delta E \ll E \), does not substantially affect the quality of the focusing. However, even in this ideal limit of a sudden potential step (i.e. \( d = 0 \) in

Figure 2. (a) Schematic view of the p–n junction forming a Veselago lens. Source \((S)\) and focal point \((F)\) are marked by open circles. Rays correspond to a perfect negative refractive index \( n = -1 \). We investigate the consequences of a finite transition width \( 2d \) (b), finite interface roughness \( \Delta x \) (c) and bulk disorder in the n- and p-regions (d).
4. Measures for focusing and collimation

In order to quantitatively characterize in the following focusing and collimation properties in realistic p–n graphene junctions we introduce as a measure for finding the electron inside the spot width ($-s, s$) of an ideal Veselago lens with $2s = \lambda_0$ (figure 3(b)) the probability

$$P(x; s) = \frac{1}{A'(x)} \int_{-s}^{s} |\psi(x,y)|^2 \, dy,$$

(7)

where the normalization constant $A(x)$ is determined by $P(x; s = W/2) = 1$. We furthermore introduce the contrast $C$,

$$C(x) = 1 - \frac{1}{A'} \left( \max(|\psi(x)|^2) - \min(|\psi(x)|^2) \right),$$

(8)

characterizing the visibility of focusing regardless of its location within the p domain. Equation (7) remains applicable also in cases where the focal point is displaced relative to the position $F$ predicted for the ideal Veselago lens. The normalization $A'$ in equation (8) will be kept fixed at $C(x) = 1$ for the ideally sharp p–n junction to allow a direct comparison between the contrast for different realizations of p–n junctions.

5. Finite transition width

As a first step towards a realistic scenario for a p–n junction we consider a finite transition (half)width of an otherwise ideal junction. We observe a gradual change from the Veselago-lens type focusing (for $2d = 0.5\,\text{nm} \ll \lambda_0$, figure 4(a)) to the low-divergence beam filter (for $2d = 15\,\text{nm} > \lambda_0$, figure 4(d)) predicted by Cheianov et al [28]. This beam shaping and collimation is not an immediate consequence of the negative trigonal warping [8, 37] become visible. Consequently, when changing from the electron to the hole cone, the conservation of $k_z$ is not perfect, leading to a slight asymmetry in the distance of focal point $F$ and source $S$ from the p–n junction.

The potential height $V_0$ provides a second tuning parameter for the p–n junction. For optimal Klein tunneling the Fermi level $E_F$ is tuned by doping to coincide with $V_0$ (figure 1). For smaller $V_0$, the increased electron wavelength decreases the resolution of the interference structures (compare figures 5(a)–(d)). Moreover, for very small $V_0$ and correspondingly large $\lambda_0$, the focal spot width increases resulting in a decrease of $P$ and $C$ (figure 5(e)). On the other hand for $V_0$ too large ($\gtrsim 0.7\,\text{eV}$), effects of the nonlinear band bending far away from the Dirac point decrease the focusing efficiency and the contrast (figure 5(e)). Simultaneously decreasing the transition width $d$, $V_0$ and $E_F$, while keeping the ratio $\lambda_0 d$ constant, improves transmission in disorder-free junctions [16]: at small energies, and thus large $\lambda_0$, a soft junction (featuring a transition length of the order of $\lambda_0$) yet large compared to the lattice constant) transmits better than a sharp one. However, experimental realizations require robustness of focusing against finite long-range disorder (as induced, e.g. by the substrate) providing a lower bound for $V_0$.

6. Disorder and interface roughness

Creating a potential step with a strong gradient in the electronic potential that varies by a fraction of an eV over a few nanometers for a p–n junction in a realistic device still poses a considerable challenge. This requires fabrication techniques beyond simple back-gate voltages, e.g. etching of contacts very close to the graphene membrane, or top-gate approaches [14]. Such approaches, however, invariably introduce some level of roughness, i.e. deviation from a straight interface perpendicular to the ribbon axis (see figure 2). Simulation of a realistic scenario for the realization of such nanoscale electron-optical structures requires the inclusion of corrugation of the p–n interface. Such interface roughness $\Delta x$ limits focusing and contrast unless it is negligibly small compared to the de Broglie wavelength $\lambda_0$. The focusing parameter $P$ and the contrast $C$ remain high for $\Delta x \lesssim \lambda_0$ but rapidly decrease for larger $\Delta x$ (figure 6(a)). Clearly, the effect of interface roughness could be reduced by increasing $\lambda_0$. The latter can be achieved by reducing the energy separation $V_0$ between the n- and p-regions. However, as the size of the focal spot also scales with $\lambda_0$, suppression of interface roughness would come at the expense of a reduced contrast.

A second limitation for a realistic graphene nanoribbon is bulk disorder, in particular due to interaction with the substrate. Disorder limits electron mobility and can cause a transport gap in quantum dot measurements [4]. To investigate the influence of such a disorder on electron-optical properties, we include a bulk disorder potential in the n- and p-regions (see figure 2(d)). We use a correlated disorder potential $V_0(\mathbf{x})$, with an amplitude $\langle V_0 \rangle$ and an autocorrelation length $\xi$ in both the n- and p-regions. A well-defined junction requires of course that local potential variations are smaller than the

$$p(\alpha) = \exp \left[ -2\pi^2 d/\lambda_0 \sin^2 \alpha \right].$$

(9)
potential step of the junction, \( V_\text{D} \ll V_0 \). As expected, the effect of disorder is strongest when the correlation length \( \xi \) matches the de Broglie wavelength, \( \xi \approx \lambda_\text{D} \), while it is reduced for both longer and shorter correlation lengths. The latter applies only as long as the correlation length is still large compared to the lattice spacing, \( \xi \ll a \). For very short correlation lengths of the order of the lattice spacing characteristic for lattice point defects, strong inter-valley scattering, a peculiarity of graphene, can severely impede well-defined electron-optical properties. It should be noted that Klein tunneling itself is not directly affected by bulk disorder but the lensing effect is. As a result, we observe several local maxima rather than a single focal point (see figure 6(b)). Accordingly, the probability \( P \) of finding the electron in the focal region is significantly reduced with increasing potential strength \( \langle V_0 \rangle \), while the contrast \( C \) decreases only slowly (see figure 6(b)). Up to a disorder potential of the order of \( \langle V_0 \rangle \approx 0.1 \text{ eV} \), the contrast is still above the 50% level. At the same time, the height of the potential step should be smaller than the characteristic energies associated with the interface corrugation,

\[
E_{\Delta x} = \hbar v_F k_{\Delta x} \quad \text{and} \quad E_d = \hbar v_F k_d
\]

with \( k_{\Delta x} = 2\pi/\Delta x \) and \( k_d = 2\pi/d \). Combining the constraints (10) and (11) provides a criterion for the admissible potential height \( V_0 \),

\[
5\langle V_0 \rangle \ll V_0 \ll \frac{1}{d + \Delta x}
\]

for which focusing and collimation should be observable. We emphasize that these bounds apply to fully phase-coherent single-electron transport.

In the present simulation we do not explicitly treat sublattice-breaking disorder \( V_\sigma \propto \sigma_z \), where the Pauli matrix \( \sigma_z \) acts
on the sublattice degree of freedom. The potential $V_c$ implies different local potentials on the two trigonal sublattices of graphene. Such short-range fluctuations are induced, e.g. by substrates such as hexagonal boron nitride. Depending on the relative alignment of the graphene layer with respect to the substrate, the two sublattices of graphene positioned, e.g. over a boron and a nitrogen atom may see quite different potentials [38]. The resulting $V_c$ opens a band gap at the Dirac point. We have verified numerically that potentials of the order of 10% of the step height $V_0$ do not strongly affect the focusing properties of the p–n junction.

Testing our predictions (equation (12)) for smaller disorder strength ($V$) and step heights $V_0$ (and thus larger wave lengths) requires larger system sizes. We simulate a junction of width $W = 300$ nm (i.e. about a factor three wider than the p–n junctions discussed above). For these simulations, we solve the Dirac equation (1) in the continuum limit rather than the TB Schrödinger equation for numerical simplicity thereby neglecting effects due to the discrete lattice structure. As expected, the small asymmetry of the transmitted wave due to trigonal warping disappears entirely. Consequently, these results can give only an upper bound for the quality of focusing for realistic graphene. We find the same qualitative trends as before: the focusing probability $P$ decreases with increasing disorder strength (figure 7). Klein collimation for larger $d$ is more robust to disorder (compare bottom and top row of figure 7). Efficient focusing at larger disorder amplitudes requires larger step heights. While larger disorder even increases the overall transmission of the p–n junction, in line with previous results [31], the focusing decreases rapidly (see figure 8).

A comparison to recent experiment further corroborates our analysis. Lee at al. realized a transition width of $d \approx 12$ nm using a top gate made of few-layer hexagonal boron nitride [27]. They consider a series of two junctions (i.e. a

Figure 6. (a) Propagated wave $|\psi_{xx}(x)|^2$ near a p–n junction of step height $V_0 = 500$ meV, width $W = 120$ nm with a rough interface $\Delta x = 5$ nm. The inset shows the evolution of focusing probability $P$ (solid line, see equation (7)) and the contrast $C$ (dashed line, see equation (8)) as a function of interface roughness $\Delta x$. (b) Same as (a) for a p–n junction with bulk disorder potential $V_D(x, V) = 0.2$ eV. The inset shows $P$ and $C$ as a function of mean disorder potential amplitude ($V$).

Figure 7. Focusing probability $P$ (equation (7)) as a function of averaged disorder strength ($V$) for three different step heights $V_0$ of the p–n junction (see insets), evaluated for a junction with narrow transition region ($d = 0.2$ nm, top row) and a wide transition region ($d = 7$ nm, bottom row). $P$ is evaluated at distance $x = 50$ nm (left column) and $x = 90$ nm (right column) from the p–n junction. Width $W$ of the ribbon is 300 nm, calculation based on the Dirac approximation of equation (1).
p–n–p and n–p–n transition), and find a small but discernible enhancement of transmission of the order of 5% due to the Veselago lens effect. Estimating the step height in this experimental device with a gate coupling $\eta \approx 7.2 \times 10^{10}$ cm$^{-2}$ V$^{-1}$ yields for a gate voltage $V_G$ of 10 V a doping level of $n = \eta V_G \approx 2.3 \times 10^{12}$ cm$^{-2}$, or a Fermi level of [27]

$$E_F = \hbar v_F \sqrt{\mu} \approx 100 \text{ meV},$$

i.e. the value used in our calculations for figure 8. The experiment estimates disorder by a mean free path $\Lambda_{\text{mfp}} \approx 1.7$ $\mu$m. To compare to the disorder scale of our calculation we determine numerically a mean free path associated with our randomly correlated disorder. We find $\Lambda_{\text{mfp}} \approx 1.7$ $\mu$m for a disorder strength of $\langle V \rangle = 20$ meV using a fit to averaged transmission coefficients [39, 40]. Our calculations yield a $P$ value of 0.45 for this disorder strength (see lowest curve in figures 7(a and c)), suggesting an upper bound for the focusing probability of two junctions of 20% in fair agreement with the experimental findings of a 5% enhancement [27].

Testing our relation for the energy scales equation (12)

$$5\langle V_0 \rangle \approx 100 \text{ meV} \lesssim V_0 \approx 100 \text{ meV} \lesssim 2\pi \hbar v_F \frac{1}{\Delta x + d} \approx 250 \text{ meV},$$

(14)

confirms that the experiment is within our suggested bounds for observing the Veselago lens effect. Indeed, the tight constraint $V_0 \leq \langle V_0 / S \rangle$ might explain the comparatively small enhancement of the transmitted current found in the experiment. We thus conclude that the quantitative bounds we provide are a good indicator for the suitability of an experimental setup to exploit electron focusing by p–n junctions.

7. Conclusions

We have investigated electron-optical focusing and filtering in realistic graphene devices generalizing the notion of a Veselago lens based on Klein tunneling of massless Dirac fermions. We find that the focusing effect is robust against moderate disorder and give quantitative upper bounds for the distortion by bulk disorder and interface roughness. The major challenge in experimental realization remains achieving sharp potential steps necessary for Klein tunneling. Comparing junctions of different step height, we find that lower step heights show better focusing for zero bulk disorder, yet suffer more strongly from finite disorder. Comparing our prediction with recent experiment indicates an optimized setting when the junction height is about an order of magnitude larger than the average bulk disorder.

Acknowledgments

We thank V Cheianov, M Katsnelson, M Morgenstern, and C Stampfer for valuable discussions. Support from the ViCoM SFB-041 are gratefully acknowledged. L A gratefully acknowledges support by FWF project 23359-N16. Numerical calculations have been performed on the Vienna Scientific Cluster (VSC2 and VSC3).

References

[14] Young A F and Kim P 2009 Nat. Phys. 5 222
[22] Pile D 2015 Nat. Photon. 9 210
[23] Landy N and Smith D R 2013 Nat. Mater. 12 25
[34] Libisch F, Stampfer C and Burgdörfer J 2009 Phys. Rev. B 79 115423