Radboud Universiteit Nijmegen

Graphene: New bridge between condensed matter physics and QED

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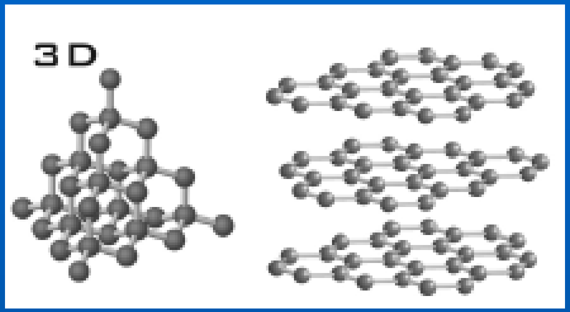
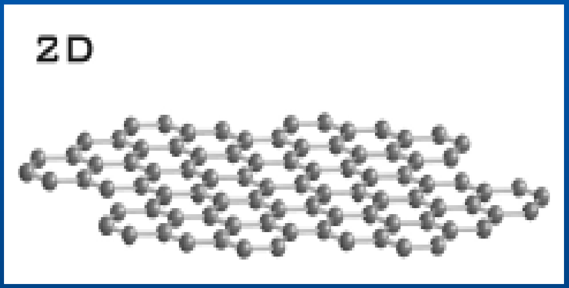
In collaboration with Andre Geim and Kostya Novoselov

Allotropes of Carbon

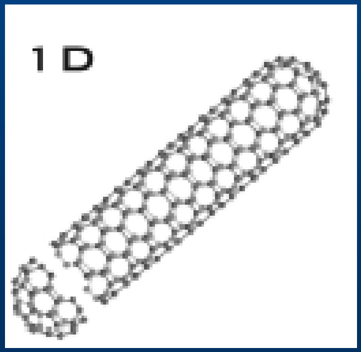
Diamond, Graphite



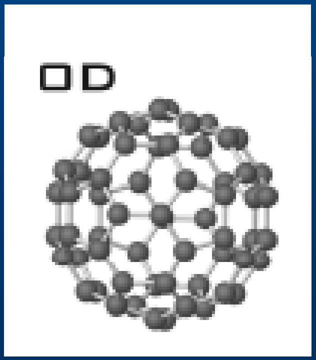
Graphene



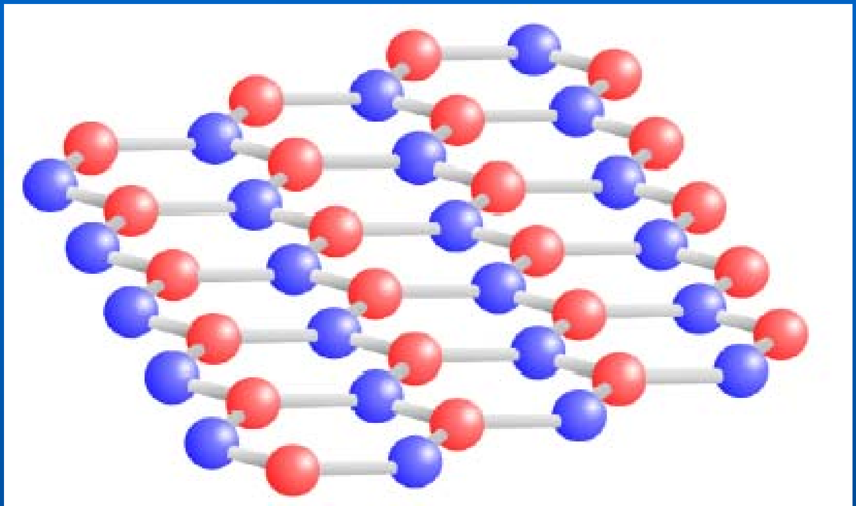
Nanotubes



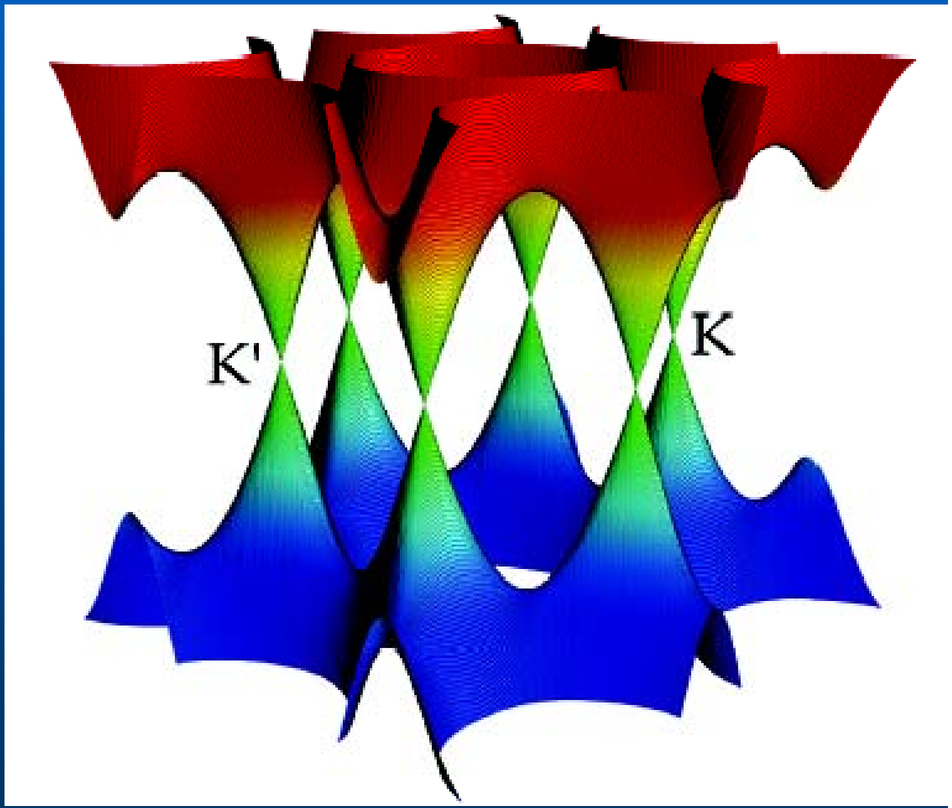
Fullerenes



Tight-binding description of the electronic structure

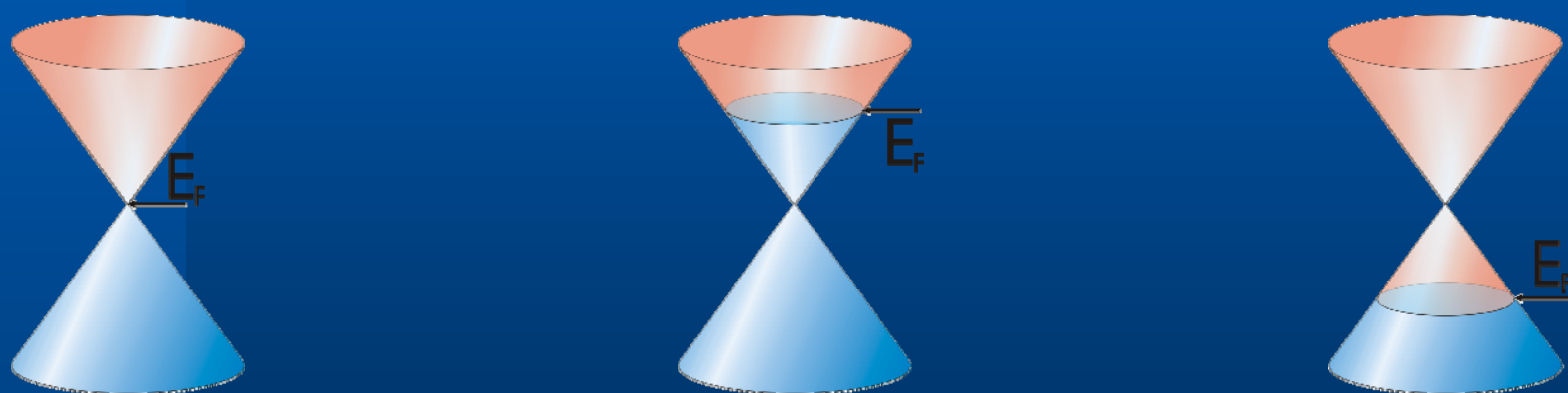


Crystal structure
of graphene:
Two sublattices



Massless Dirac fermions

Spectrum near *K* (*K'*) points is linear. Conical cross-points: provided by symmetry and thus robust property



Undoped | Electron | Hole

Massless Dirac fermions II

If Umklapp-processes K-K' are neglected:
2D Dirac massless fermions with the Hamiltonian

$$H = -i\hbar c^{*} \begin{pmatrix} 0 & \frac{\partial}{\partial x} - i\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} & 0 \end{pmatrix} \qquad \hbar c^{*} = \frac{\sqrt{3}}{2}\gamma_0 a$$

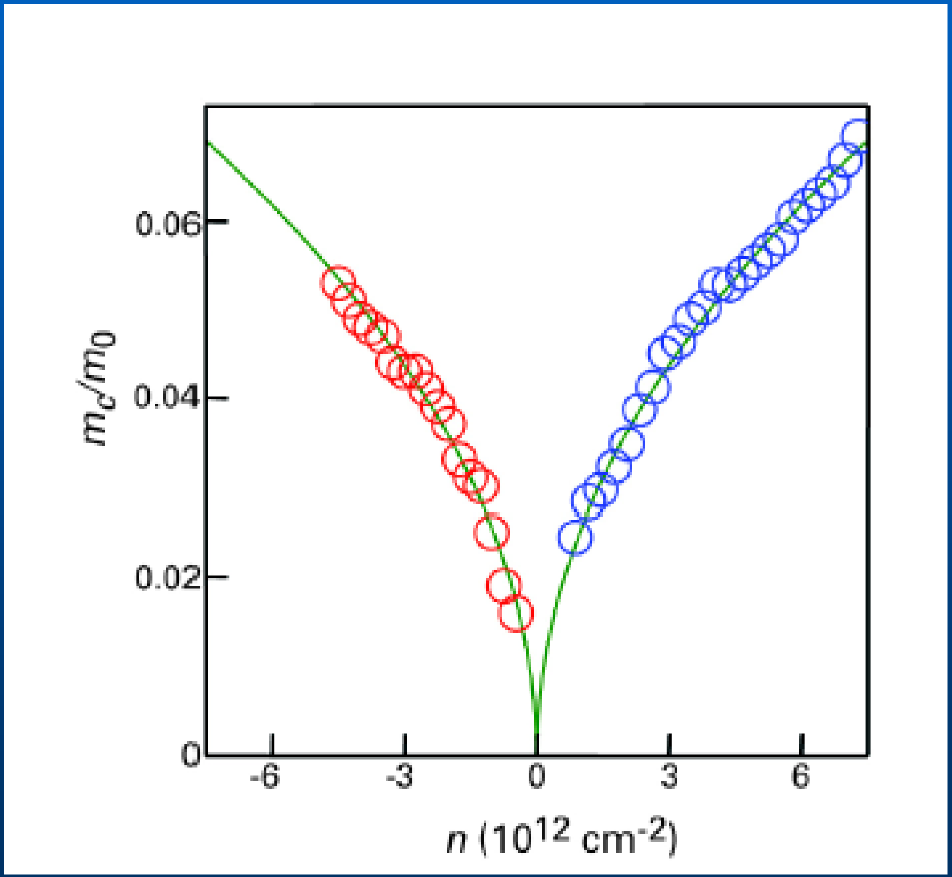
"Spin indices" label sublattices *A* and *B* rather than real spin

Experimental confirmation: Schubnikov – de Haas effect + anomalous QHE

K. Novoselov et al, Nature 2005;

Y. Zhang et al, Nature 2005

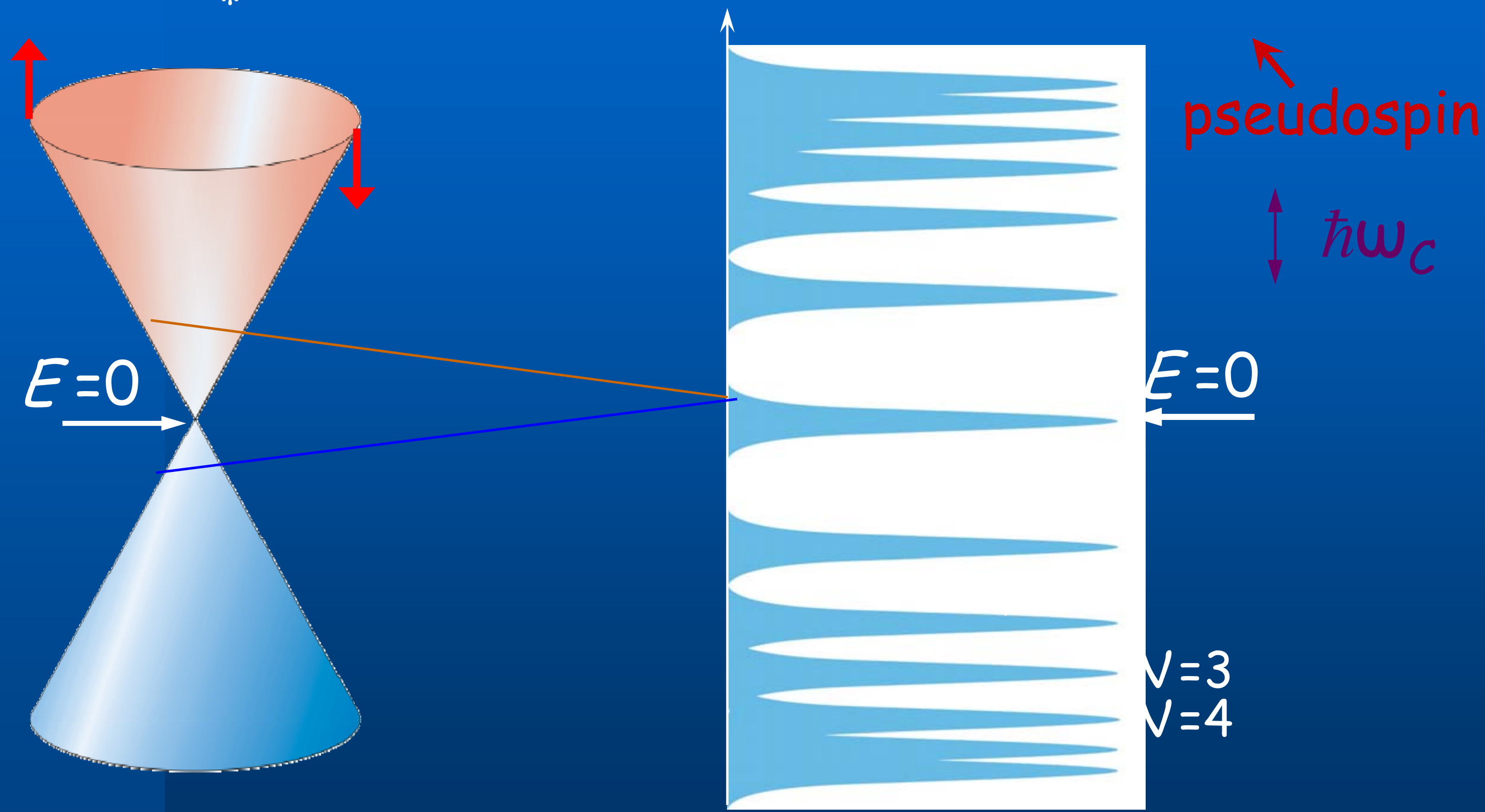
Square-root dependence of the cyclotron mass on the charge-carrier concentration



Anomalous Quantum Hall Effect

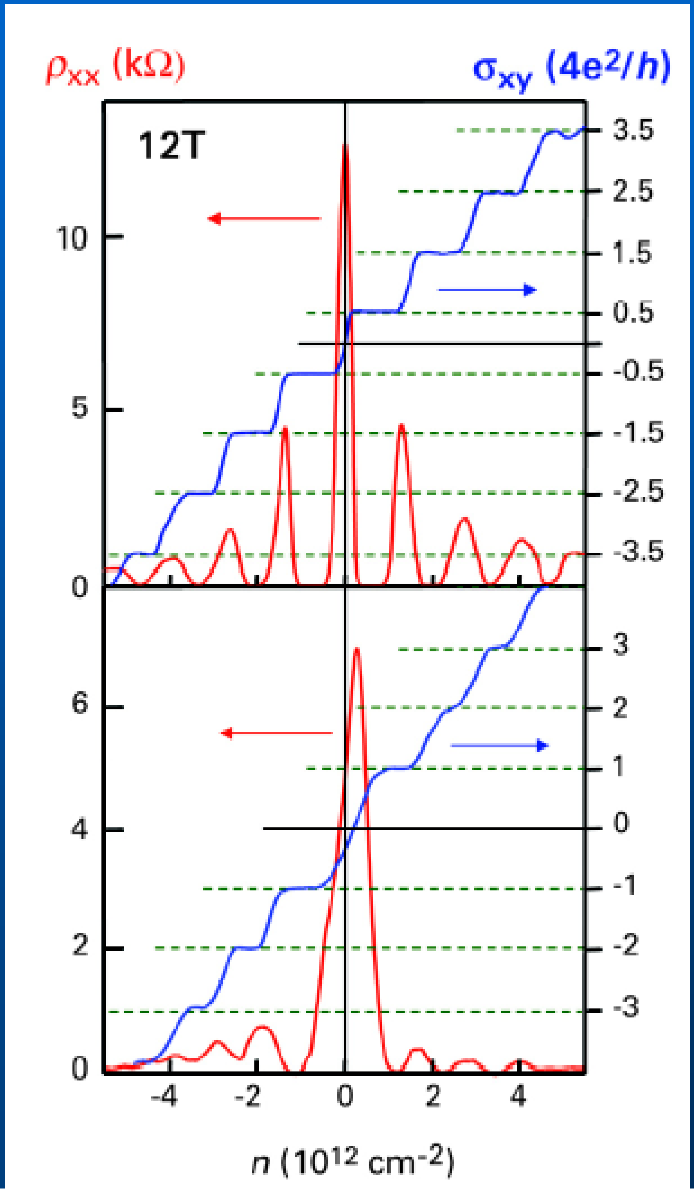
$E = \hbar c_* k$

$E_N = [2 e\hbar c_*^2 B(N + \frac{1}{2} \pm \frac{1}{2})]^{1/2}$



The lowest Landau level is *at ZERO energy* and shared equally by electrons and holes

Anomalous QHE in single- and bilayer graphene



Single-layer: half-integer quantization since zero-energy Landau level has twice smaller degeneracy

Bilayer: integer quantization but no zero-*v* plateau (chiral fermions with parabolic gapless spectrum)

Half-integer quantum Hall effect and "index theorem"

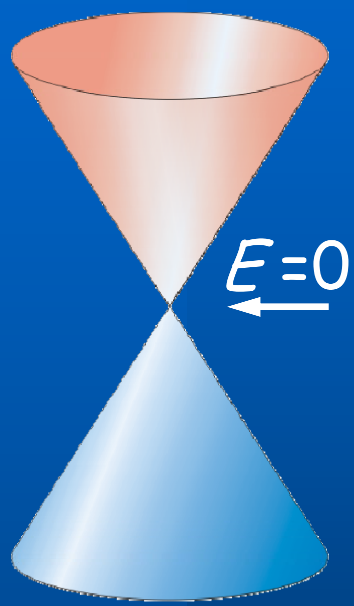
Atiyah-Singer index theorem: number of chiral modes with zero energy for massless Dirac fermions with gauge fields

Simplest case: 2D, electromagnetic field

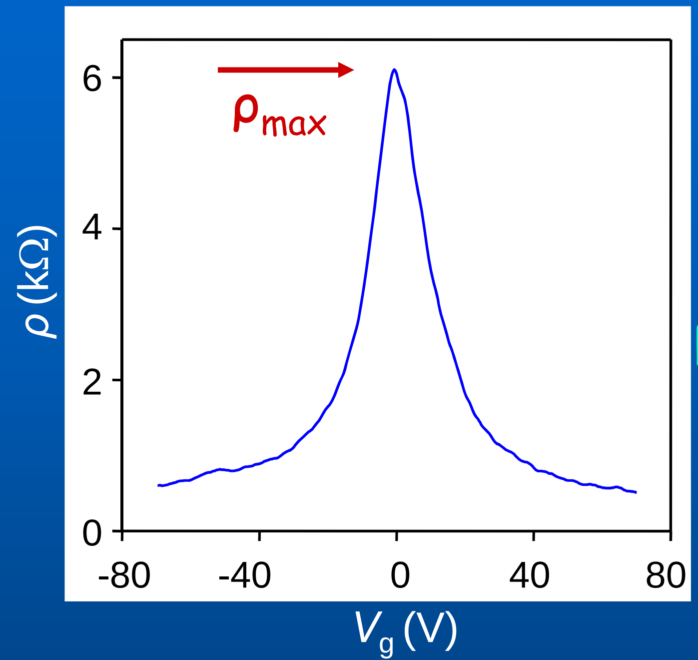
$$N_+ - N_- = \phi / \phi_0$$

(magnetic flux in units of the flux quantum)

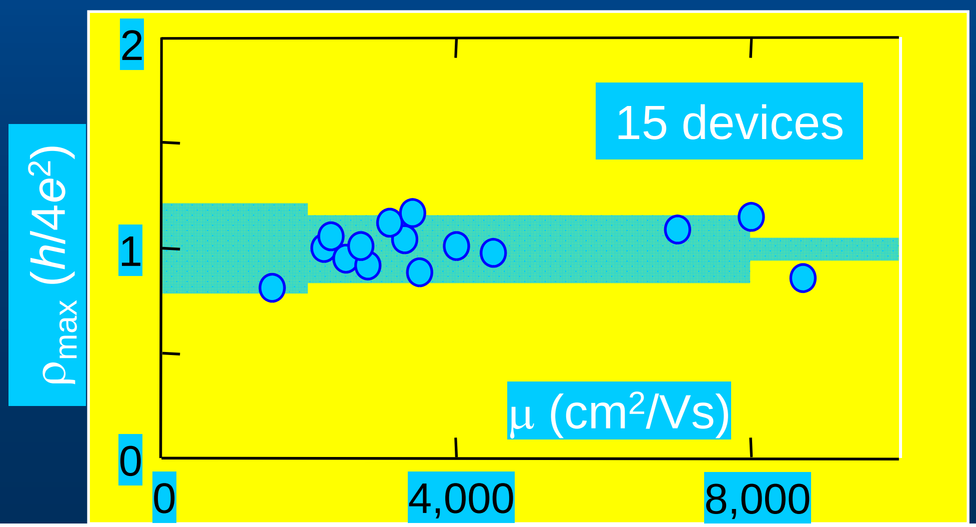
Quantum-Limited Resistivity



zero-gap semiconductor



no temperature dependence in the peak between 3 and 80K



Problem of minimal conductivity

At zero doping there is a finite minimal conductivity approximately e^2/h per channel

(do not mix with conductance quantization in ballistic regime)

Amazing property of 2D massless particles: finite conductivity for ideal crystal – no scattering, no current carriers!

Landauer formula approach

Conductance = $e^2/h \, Tr \, T$ per valley per spin

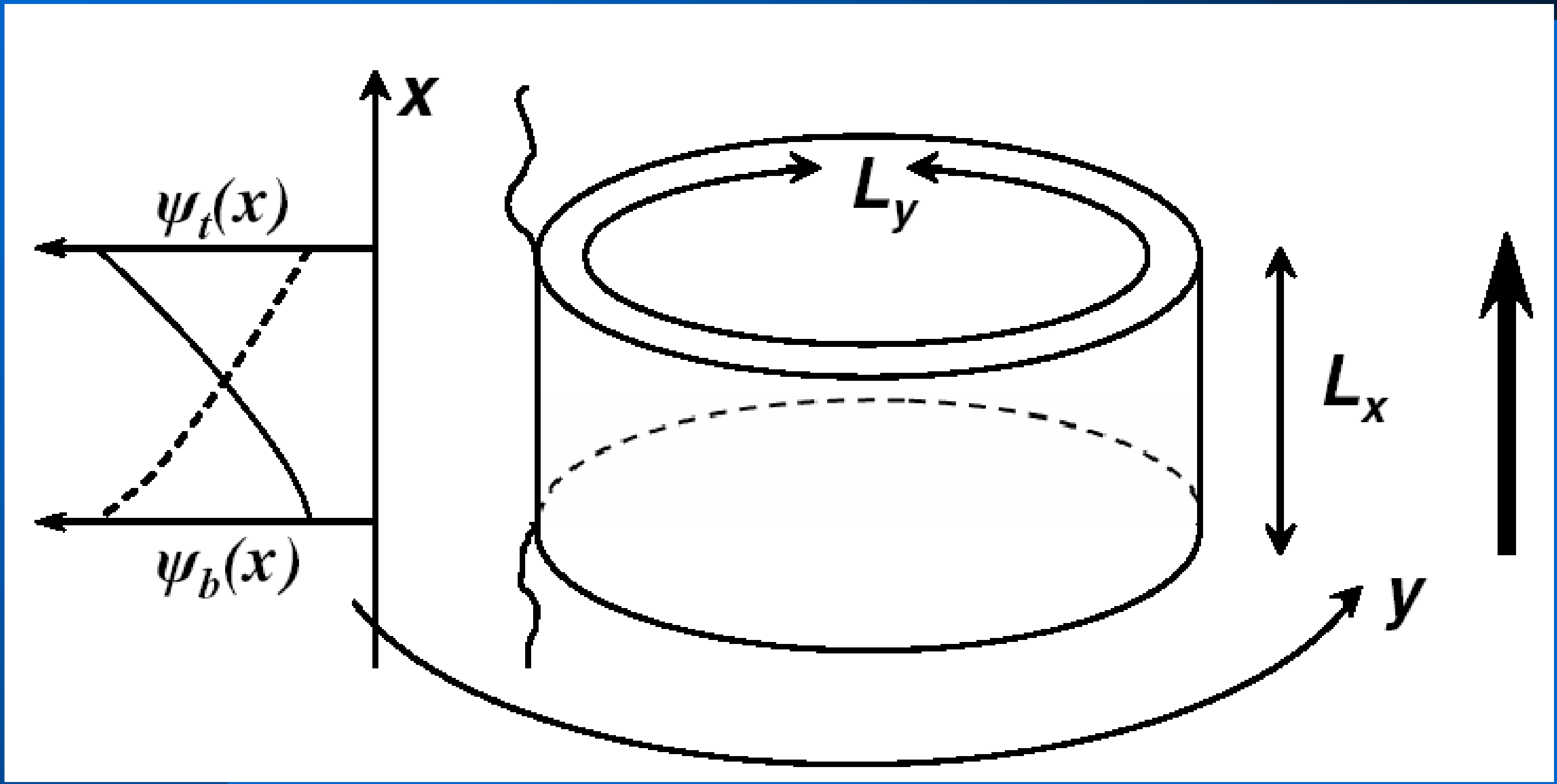
T is the transmission probability matrix

The wave functions of massless Dirac fermions at zero energy:

$$\left(\frac{\partial}{\partial x} \pm i \frac{\partial}{\partial y}\right)\psi_{\pm}(x,y) = 0 \qquad \psi_{\pm}(x,y) = f(x \pm iy) \quad \forall f$$

Boundary conditions determine the functions f

Landauer formula II



$f(y+L_y) = f(y)$

$$\psi_\pm(x,y) = \exp\left[i\frac{2\pi n}{L_y}(x \pm iy)\right] \qquad n = 0, \pm 1, \pm 2, \ldots$$

Edge states near the top and bottom of the sample

Landauer formula III

Leads from doped graphene

$$T_n = |t(k_y)|^2 = \frac{\cos^2\phi}{\cosh^2(k_y L_x) - \sin^2\phi}$$

$$\sin\phi = k_y / k_F$$

$$TrT = \sum_{n=-\infty}^{\infty} \frac{1}{\cosh^2(k_y L_x)} \simeq \frac{L_y}{\pi L_x}$$

Conductivity per channel: $e^2/(\pi h)$

The problem of “missing pi(e)”!

Minimal conductivity and Zitterbewegung

For Dirac particles the current operator does not commute with the Hamiltonian of free-motion

$$\mathbf{j}(t) = \mathbf{j}_0(t) + \mathbf{j}_1(t) + \mathbf{j}_1^\dagger(t)$$

$$\mathbf{j}_0(t) = ev \sum_{\mathbf{p}} \Psi_{\mathbf{p}}^\dagger \frac{\mathbf{p}(\mathbf{p}\sigma)}{p^2} \Psi_{\mathbf{p}}$$

$$\mathbf{j}_1(t) = \frac{ev}{2} \sum_{\mathbf{p}} \Psi_{\mathbf{p}}^\dagger \left[\sigma - \frac{\mathbf{p}(\mathbf{p}\sigma)}{p^2} + \frac{i}{p} \sigma \times \mathbf{p} \right] \Psi_{\mathbf{p}} e^{2i\epsilon_{\mathbf{p}} t}$$

The reason: indeterminacy of the electron coordinate and electron-hole pair creation at the electron motion

$\epsilon_{\mathbf{p}} = vp/\hbar$ is the particle frequency

Minimal conductivity and Zitterbewegung II

Kubo formula for conductivity

$$\sigma(\omega) = \frac{1}{2A} \int_0^\infty dt e^{i\omega t} \int_0^\beta d\lambda \left\langle \mathbf{j}(t - i\lambda)\, \mathbf{j} \right\rangle$$

Indeterminacy 0•∞ due to Zitterbewegung

Resulting static conductivity of order of e^2/h

Chiral tunneling and Klein paradox

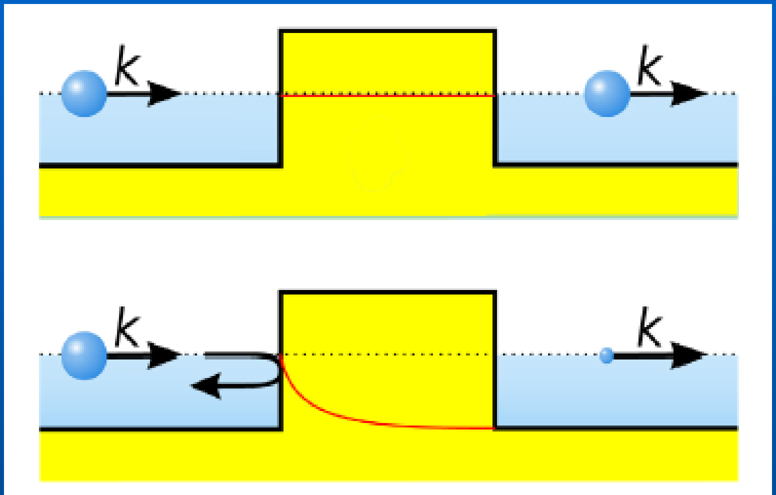
Electronics: heterostructures (*p*-*n*-*p* junctions etc.)

Classical particles: cannot propagate through potential barriers
Quantum particles: can propagate (tunneling) but probability decays exponentially with barrier height and width
Ultrarelativistic quantum particles: can propagate with the probability of order of unity (Klein paradox)

Klein paradox II

Ultrarelativisic

Nonrelativistic



Tunnel effect: momentum and coordinate are complementary variables, kinetic and potential energy are not measurable simultaneously

Relativistic case: even the *coordinate itself* is not measurable, particle-antiparticle pair creation

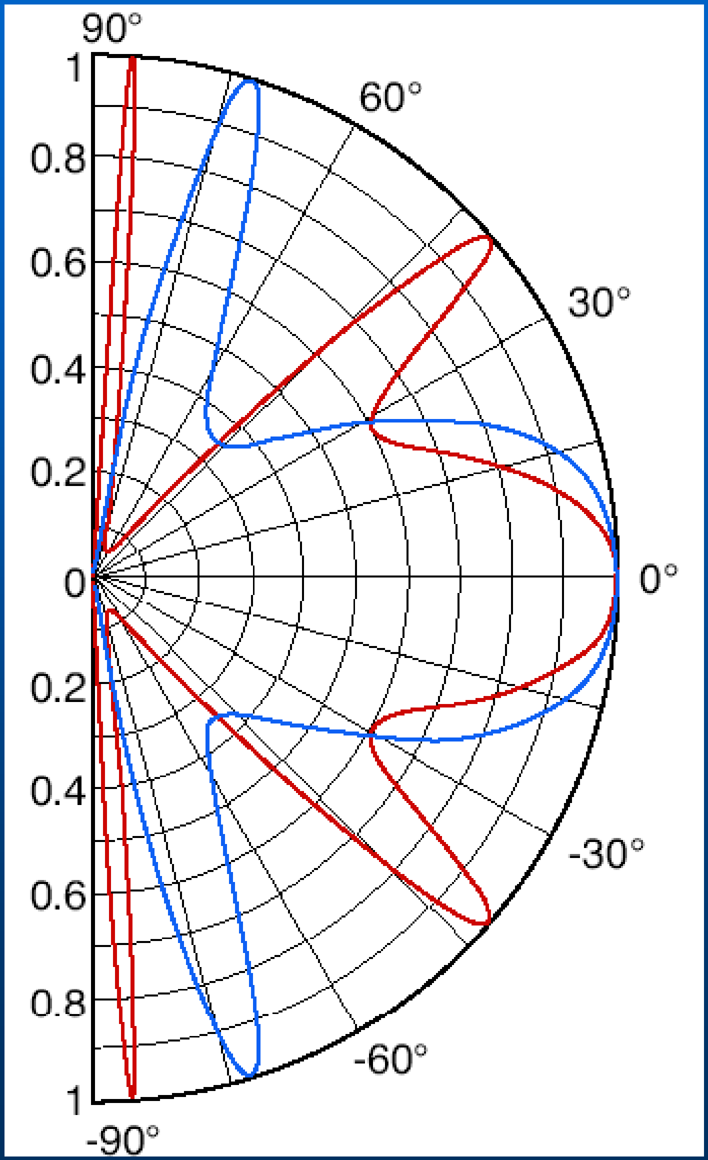
Klein paradox III

Transmission probability

Barrier width 100 *nm*

Electron concentration outside barrier 0.5×10^{12} cm^{-2}

Hole concentration inside barrier 1×10^{12} cm^{-2} (red) and 3×10^{12} cm^{-2} (blue)

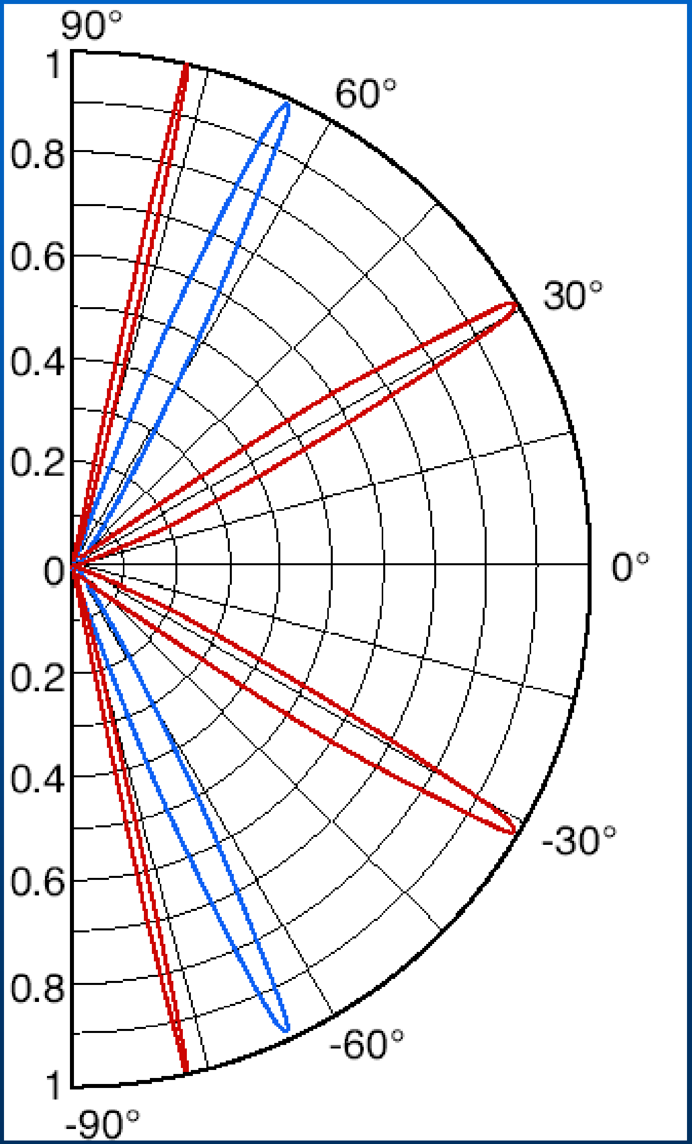


Klein paradox IV

A problem: graphene transistor can hardly be locked!

Possible solution: use bilayer graphene: chiral fermions with parabolic spectrum – no analogue in particle physics!

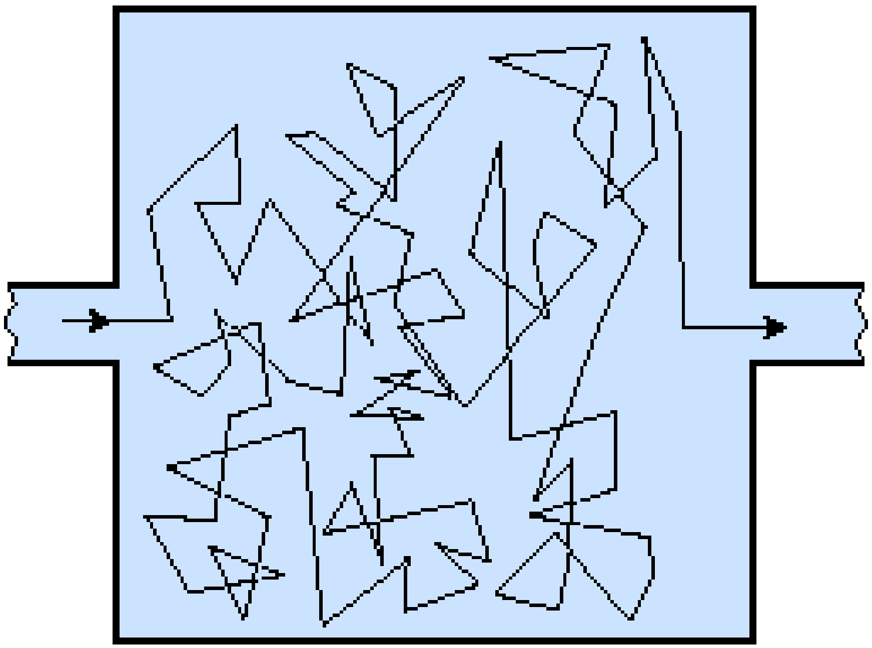
Transmission for bilayer; parameters are the same as for previous slide



Klein paradox and the absence of localization

Back scattering is forbidden for chiral fermions!

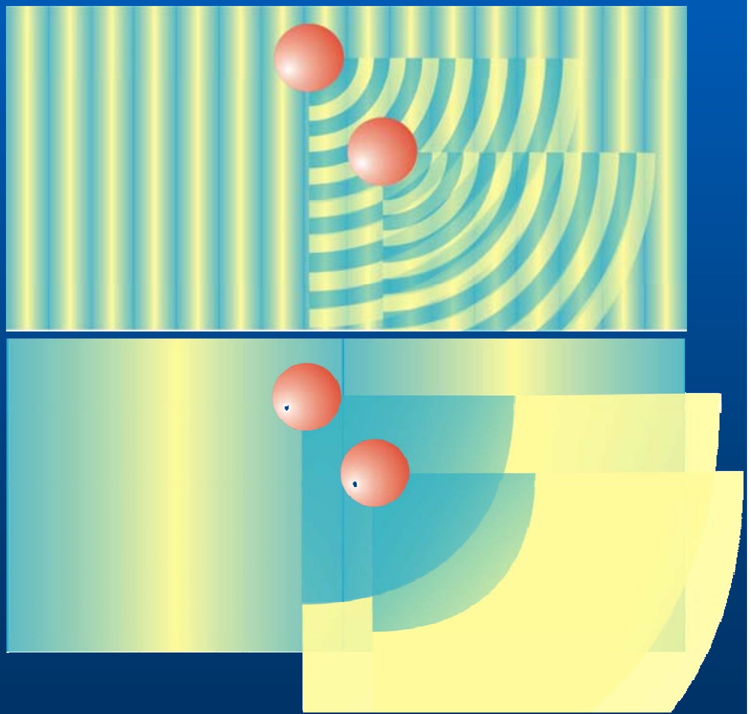
Unusual transport properties



Electrons cannot be locked by random potential relief neither for singe-layer nor for bilayer graphene – absence of localization and minimal conductivity?

Quantum-Limited Resistivity

$$\sigma = ne\mu = \frac{e^2}{h} k_F l$$

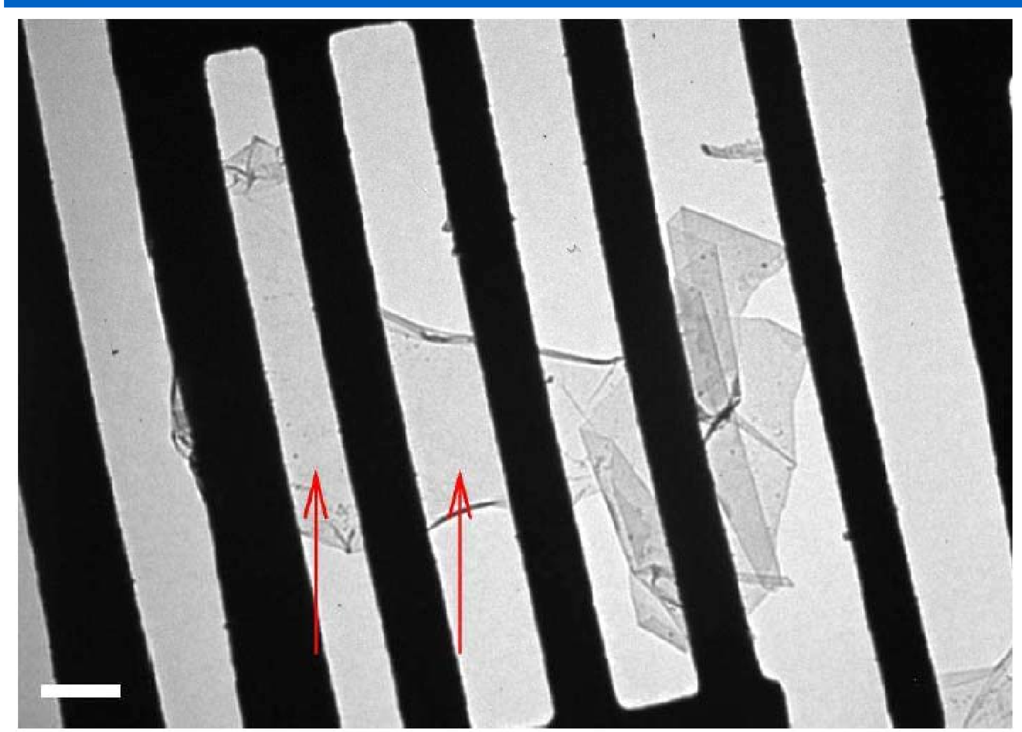


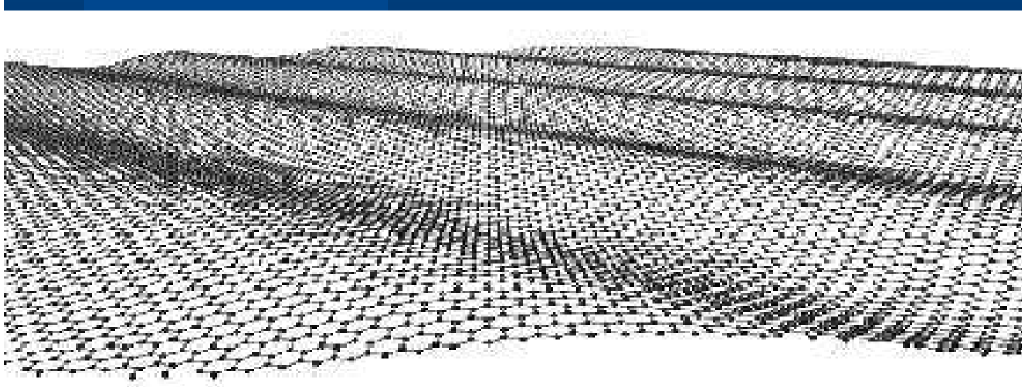
Mott's argument: $l \geq \lambda_F$

$$\sigma \geq \frac{e^2}{h}$$

(in the absence of localization)

Ripples on graphene: Dirac fermions in curved space





Freely suspended graphene membrane (J. C. Meyer et al, to appear in *Nature*)

2D crystals in 3D space cannot be flat, due to bending instability

Random shifts of Dirac points: gauge field acting on electrons

Suppression of weak localization…

Pseudomagnetic fields due to ripples

Deformation tensor in the plane

$$\overline{u}_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i}\frac{\partial u_k}{\partial x_j} + \frac{\partial h}{\partial x_i}\frac{\partial h}{\partial x_j}\right)$$

$x_i = (x, y)$ **coordinates in the plane**

u_i **displacement vector**

h **displacements normal to the plane**

Pseudomagnetic fields II

Nearest-neighbour approximation: changes of hopping integrals

$$\gamma = \gamma_0 + \left(\frac{\partial \gamma}{\partial \overline{u}_{ij}} \right)_0 \overline{u}_{ij}$$

$$H = v_F \sigma \left(-i\hbar\nabla - \frac{e}{c}\mathcal{A} \right)$$

"Vector potentials"

$$\mathcal{A}_x = \frac{c}{2ev_F}\left(\gamma_2 + \gamma_3 - 2\gamma_1\right),$$
$$\mathcal{A}_y = \frac{\sqrt{3}c}{2ev_F}\left(\gamma_3 - \gamma_2\right),$$

K **and** ***K'*** **points are shifted in opposite directions; Umklapp processes restore time-reversal symmetry**

Relativistic effects and scattering mechanisms in graphene

- **Weakening of scattering by finite-radius potentials for massless Dirac fermions in comparison with normal 2D electron gas**
- **“Vacuum polarization” effects (electron-hole pair creation near charge impurities) and strong nonlinear screening**

Scattering by point defects: Contribution to transport properties

Contribution of point defects to resistivity *ρ*

$$\rho = \frac{2}{e^2 v_F^2 N(E_F)} \frac{1}{\tau(k_F)},$$

$$\frac{1}{\tau(k_F)} = n_{imp} v_F \int_0^{2\pi} d\phi \frac{d\sigma(\phi)}{d\phi} (1 - \cos\phi)$$

Radial Dirac equation

$$\frac{df_l(r)}{dr} + \frac{l+1}{r} f_l(r) - \frac{i}{\hbar v_F} [E - V(r)] g_l(r) = 0$$

$$\frac{dg_l(r)}{dr} - \frac{l}{r} g_l(r) - \frac{i}{\hbar v_F} [E - V(r)] f_l(r) = 0.$$

where $l = 0, \pm 1, \ldots$ is the angular-momentum quantum number, $g_l(r)\, e^{il\phi}$ and $f_l(r)\, e^{i(l+1)\phi}$ are components of Dirac pseudospinor; to be specific we will consider the case of electrons $E = \hbar v_F k > 0$.

Scattering cross section

Wave functions beyond the range of action of potential

$$g_l(r) = A\left[J_l(kr) + t_l H_l^{(1)}(kr)\right],$$

$$f_l(r) = iA\left[J_{l+1}(kr) + t_l H_{l+1}^{(1)}(kr)\right]$$

Scattering cross section:

$$\frac{d\sigma(\phi)}{d\phi} = \frac{2}{\pi k}\left|\sum_{l=-\infty}^{\infty} t_l e^{il\phi}\right|^2$$

Scattering cross section II

Exact symmetry for massless fermions:

$$f \longleftrightarrow g, l \longleftrightarrow -l-1 \text{ which means } t_l = t_{-l-1}$$

As a consequence

$$\frac{d\sigma(\phi)}{d\phi} = \frac{2}{\pi k}\left|\sum_{l=0}^{\infty} t_l \cos\left[(l+1/2)\phi\right]\right|^2$$

The back scattering ($\phi = \pi$) is absent rigorously

Scattering cross section II

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Cylindrical potential well

$V(r) = V_0$ at $r < R$ and $V(r) = 0$ otherwise

continuity of the wave functions at $r = R$

$$t_l(k) = \frac{J_l(qR)\,J_{l+1}(kR) - J_l(kR)\,J_{l+1}(qR)}{H_l^{(1)}(kR)\,J_{l+1}(qR) - J_l(qR)\,H_{l+1}^{(1)}(kR)}$$

$$q = (E - V_0)/\hbar v_F$$

Small energy case kR « 1

$$t_l(k) \simeq \frac{\pi i}{(l!)^2} \frac{J_{l+1}(qR)}{J_l(qR)} \left(\frac{kR}{2}\right)^l$$

s-scattering $(l = 0)$ dominates

Estimation of the resistivity

$$\rho \simeq (h/4e^2)\, n_{imp} R^2$$

Resonant scattering case

$$J_0(qR) = 0$$

Much larger resistivity

$$\rho \simeq \frac{h}{4e^2}\frac{n_{imp}}{n}\ln^2(k_F R)$$

Nonrelativistic case:

$$t_l(k) = \frac{(k/q)\,J_l(qR)\,J_{l+1}(kR) - J_l(kR)\,J_{l+1}(qR)}{H_l^{(1)}(kR)\,J_{l+1}(qR) - (k/q)\,J_l(qR)\,H_{l+1}^{(1)}(kR)}$$

The same result as for resonant scattering for massless Dirac fermions!

Charge impurities

Coulomb potential

$$V_0\left(\mathbf{r}\right) = \frac{Ze^2}{\epsilon r}$$

Scattering cross section *σ* is proportional to 1/*k*, leading term to resistivity (concentration independent mobility)

(Nomura & MacDonald, PRL 2006;
Ando, JPSJ 2006 – linear screening theory)

Nonlinear screening

MIK, PR B 74, 201401(R) (2006)

Rigorous expression for total potential

$$V(\mathbf{r}) = V_0(\mathbf{r}) + V_{ind}(\mathbf{r})$$

$$V_{ind}(\mathbf{r}) = \frac{e^2}{\epsilon} \int d\mathbf{r}' \frac{n(\mathbf{r}') - \overline{n}}{|\mathbf{r} - \mathbf{r}'|} + V_{xc}(\mathbf{r})$$

Thomas-Fermi theory

$$V_{ind}(\mathbf{r}) = \frac{e^2}{\epsilon} \int d\mathbf{r}' \frac{n[\mu - V(\mathbf{r}')] - n(\mu)}{|\mathbf{r} - \mathbf{r}'|}$$

$$n(\mu) = \frac{1}{\pi} \frac{\mu |\mu|}{\hbar^2 v_F^2}$$

Suppression of the screening

Effective impurity charge

$$Z^* \simeq \frac{Z}{1 + ZQ \ln \frac{1}{\kappa a}}$$

Inverse linear screening radius

$$\kappa = \frac{4e^2 |\mu|}{\epsilon \hbar^2 v_F^2}$$

A very strong suppression: tens of times

Main scattering mechanism

Experimentally: mobility is approximately concetration independent but is rather weakly sensitive to adding of charge impurities

Nonlinear screening: a controversial issue (Thomas-Fermi theory beyond formal limit of its applicability)

A hypothesis: scattering by ripples

Main scattering mechanism II

Scattering by random vector potential:

$$\frac{1}{\tau} \simeq \frac{2\pi}{\hbar} N\left(E_F\right) \left\langle \mathbf{V_q V_{-q}} \right\rangle_{q \simeq k_F}$$

Random potential due to surface curvature

$$\left\langle \mathbf{V_q V_{-q}} \right\rangle \simeq \left(\frac{\hbar v_F}{a}\right)^2 \sum_{\mathbf{q}_1 \mathbf{q}_2} \left\langle h_{\mathbf{q}-\mathbf{q}_1} h_{\mathbf{q}_1} h_{-\mathbf{q}+\mathbf{q}_2} h_{-\mathbf{q}_2} \right\rangle \left[\left(\mathbf{q}-\mathbf{q}_1\right)\mathbf{q}_1\right]\left[\left(\mathbf{q}-\mathbf{q}_2\right)\mathbf{q}_2\right]$$

Assumption: intrinsic ripples due to thermal fluctuations

Main scattering mechanism III

Harmonic approximation

$$\langle h_{\mathbf{q}} h_{-\mathbf{q}} \rangle = \frac{T}{\kappa q^4}$$

Small *q*: anharmonic coupling of bending and stretching phonons (D. Nelson et. al.)

$$\langle h_{\mathbf{q}} h_{-\mathbf{q}} \rangle = \frac{1}{q^4} \left(\frac{q}{q_0} \right)^{\eta}$$

Crossover wave vector:

$$\eta \simeq 0.8$$

$$q^* = q_0 \left(\frac{T}{\kappa} \right)^{1/\eta}$$

Main scattering mechanism IV

Ripples quenched at room temperature:

$$q^* \simeq 10^{-2}/a$$

For the case

$$k_F \geq q^*$$

$$\rho \simeq \frac{h}{4e^2} \frac{(q_0 T/\kappa)^2}{n}$$

The same concentration dependence as for charge impurities

Conclusions and final remarks

- **Relativistic effects are of crucial importance for graphene physics and applications (minimal conductivity, absence of localization, carbon transistors…)**
- **Exotic phenomena in everyday's life (e.g., Klein paradox)**
- **Some interesting physics beyond particle physics (e.g., bilayer – chiral fermions with parabolic spectrum**
- **Important: "finite-structure constant" is larger than 1 (e.g., strong suppression of Coulomb potential due to "nulification")**