Radboud Universiteit Nijmegen

Graphene: New bridge between condensed matter physics and QED

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Outline

1. Introduction

2. Ripples: Dirac fermions in curved space

3. Anomalous Quantum Hall Effect

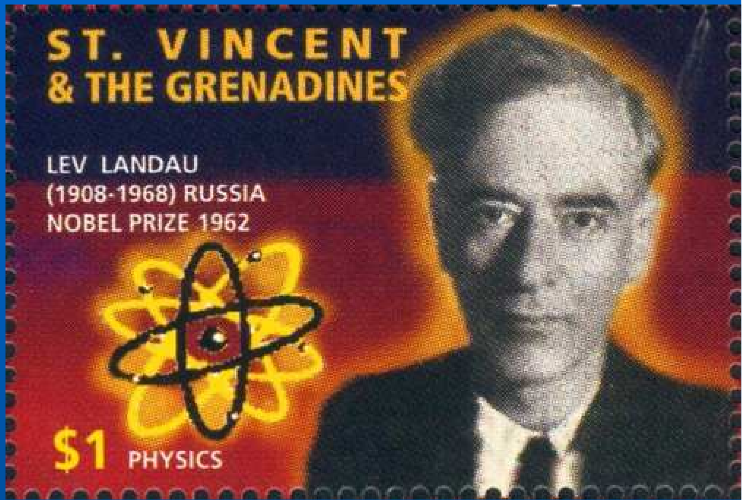
4. Problem of minimal conductivity and Zitterbewegung

5. Chiral tunneling and Klein paradox

6. Vacuum polarization of supercritical charges

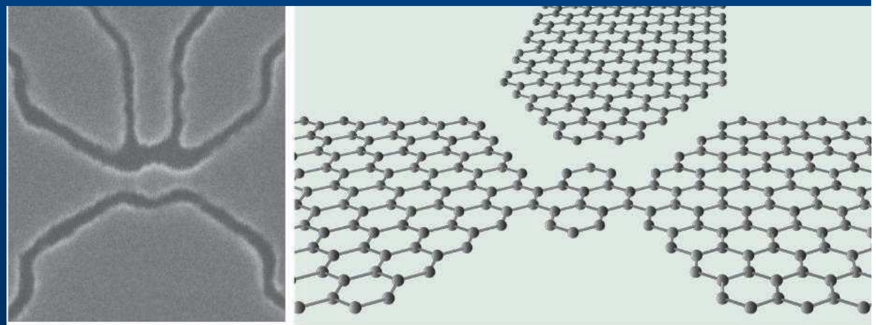
Landau and graphene

Unity of theoretical physics



Landau levels: Shubnikov-de Haas, QHE

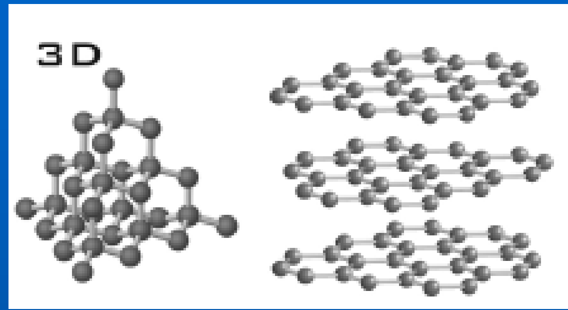
Landau and Peierls: quantum relativistic mechanics is not a mechanics



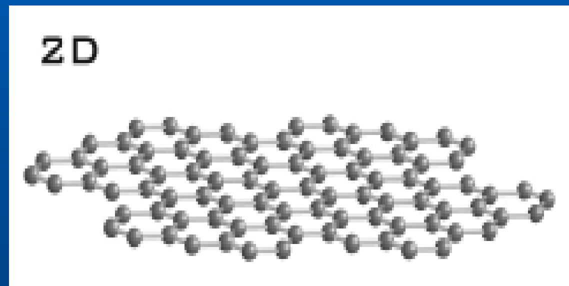
Landau and Pomeranchuk: “Moscow zero”

Allotropes of Carbon

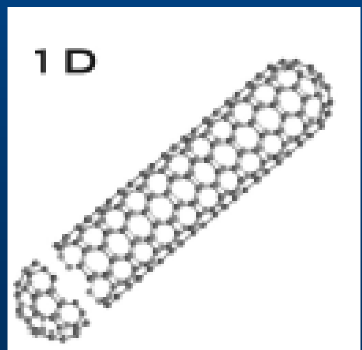
Diamond, Graphite



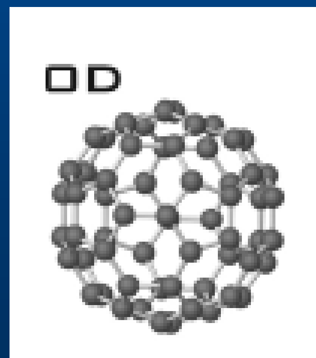
Graphene: prototype truly 2D crystal



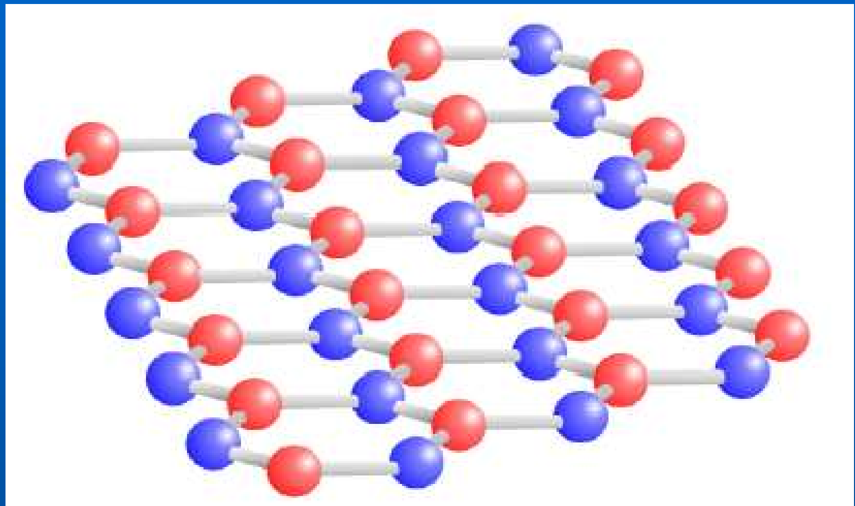
Nanotubes



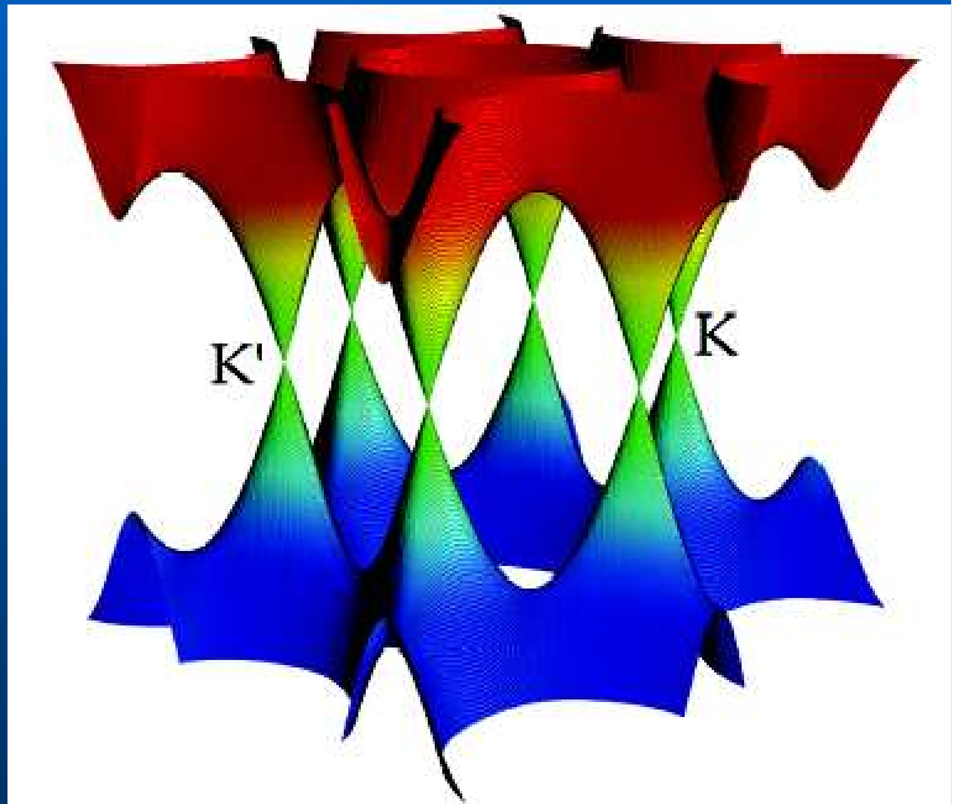
Fullerenes



Tight-binding description of the electronic structure

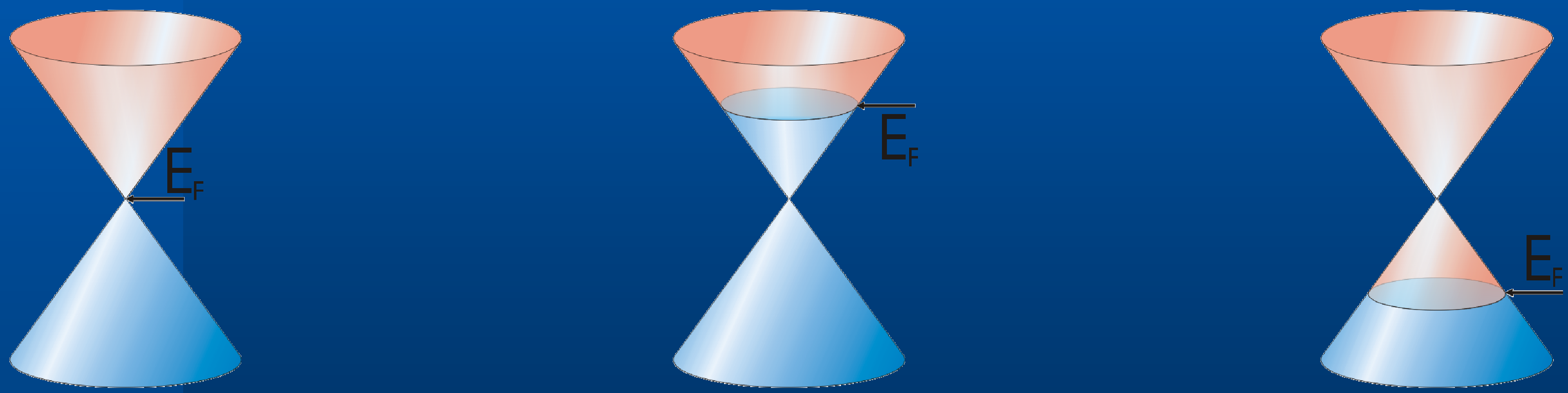


Crystal structure
of graphene:
Two sublattices



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

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

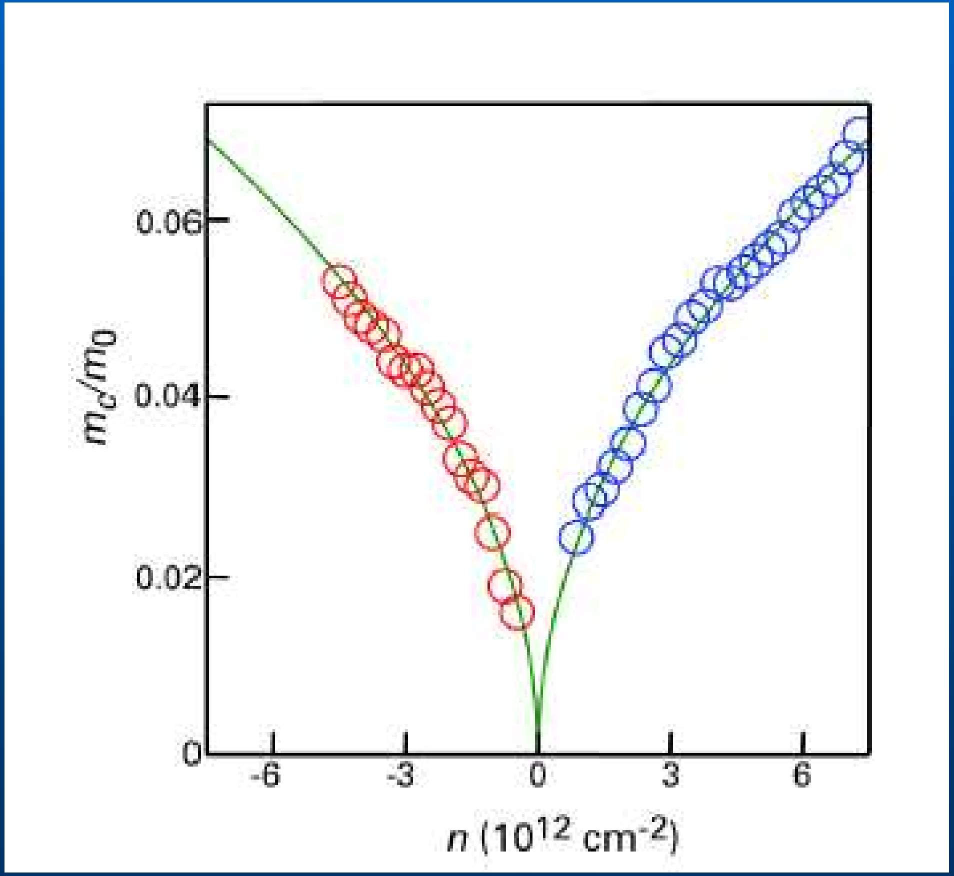
"Spin indices'' label sublattices *A* and *B*
rather than real spin

Experimental confirmation: Schubnikov – de Haas effect + anomalous QHE

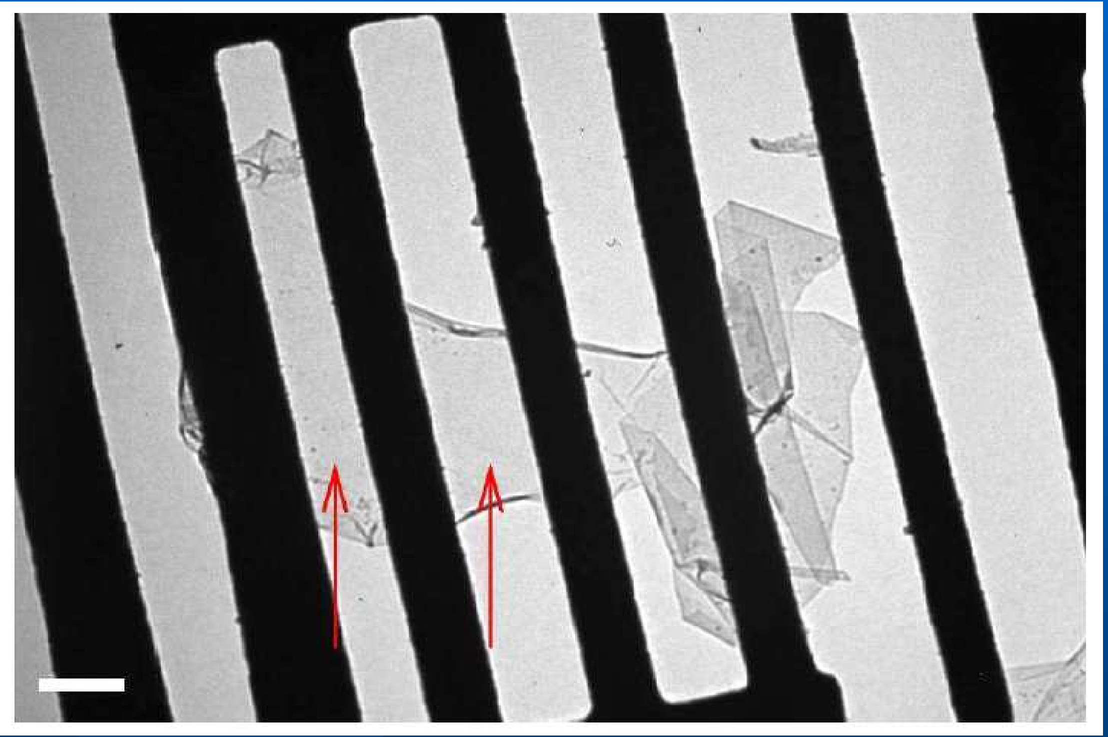
K. Novoselov et al, Nature 2005;
Y. Zhang et al, Nature 2005

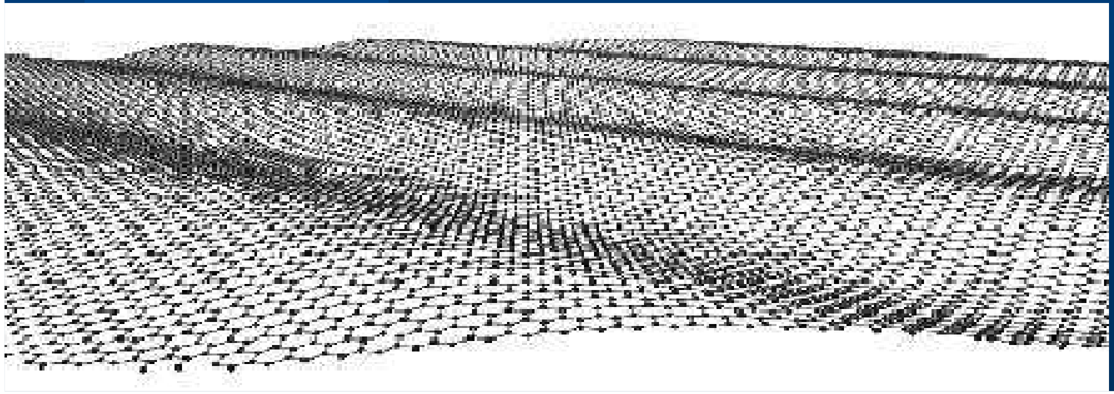
Square-root dependence of the cyclotron mass on the charge-carrier concentration

+ anomalous QHE ("Berry phase")



Ripples on graphene: Dirac fermions in curved space





Freely suspended graphene membrane is partially crumpled

J. C. Meyer et al, *Nature 446, 60 (2007)*

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

Computer simulations

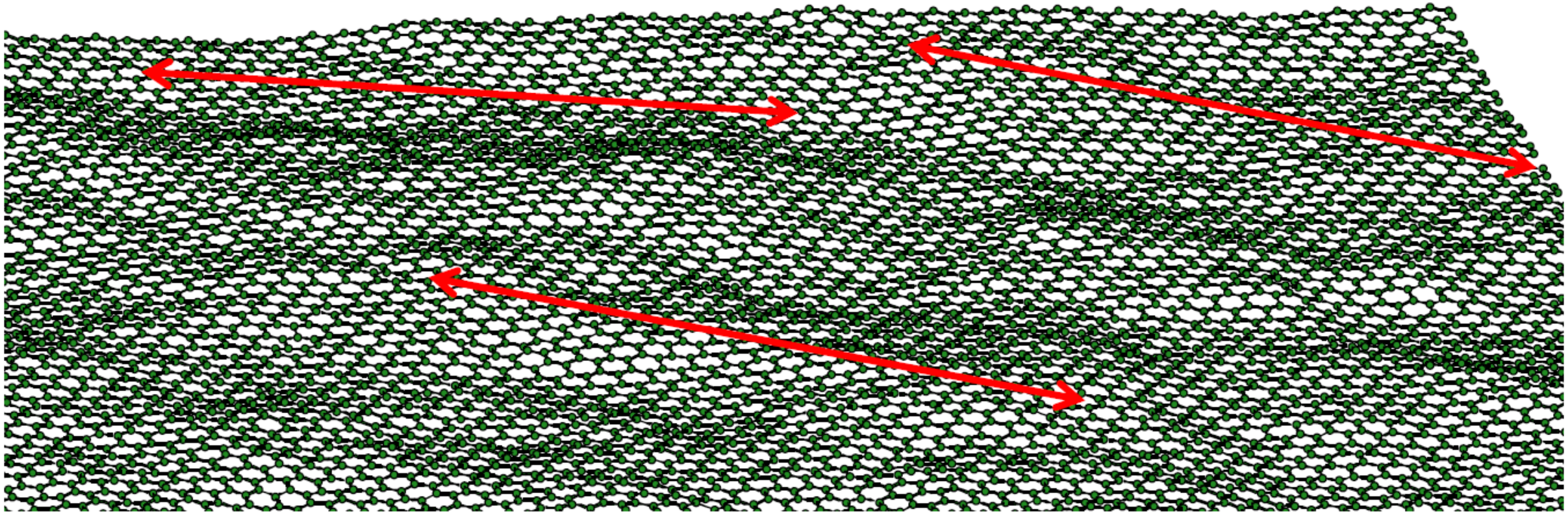
(Fasolino, Los & MIK, Nature Mater., Nov.2007)

Bond order potential for carbon: LCBOPII (Fasolino & Los 2003): fitting to energy of different molecules and solids, elastic moduli, phase diagram, thermodynamics, etc.

Method: classical Monte-Carlo, crystallites with N = 240, 960, 2160, 4860, 8640, and 19940

Temperatures: 300 K , 1000 K, and 3500 K

A snapshot for room temperature



The red arrows are 70 Å long

Broad distribution of ripple sizes + some typical length due to intrinsic tendency of carbon to be bonded

Chemical bonds I

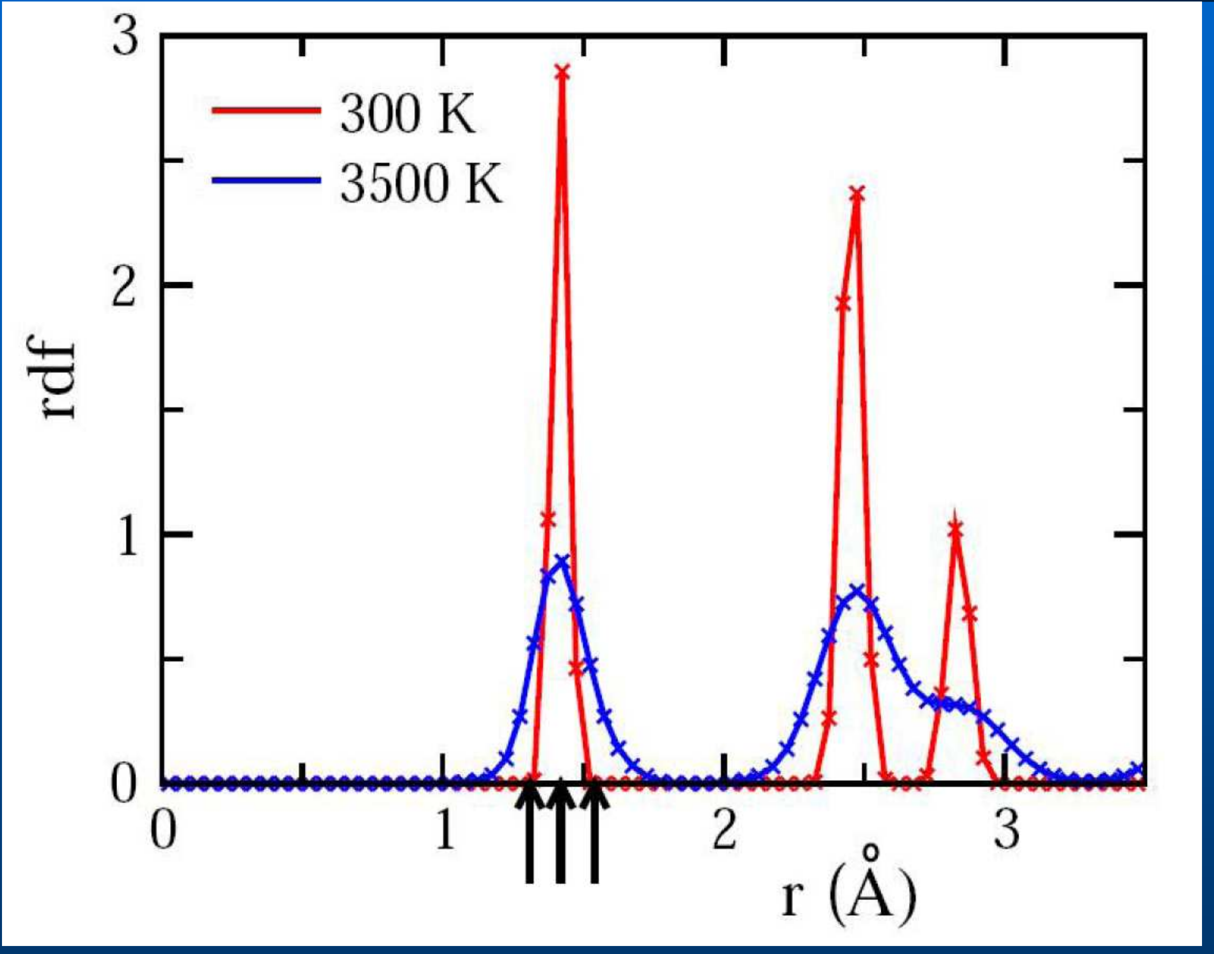
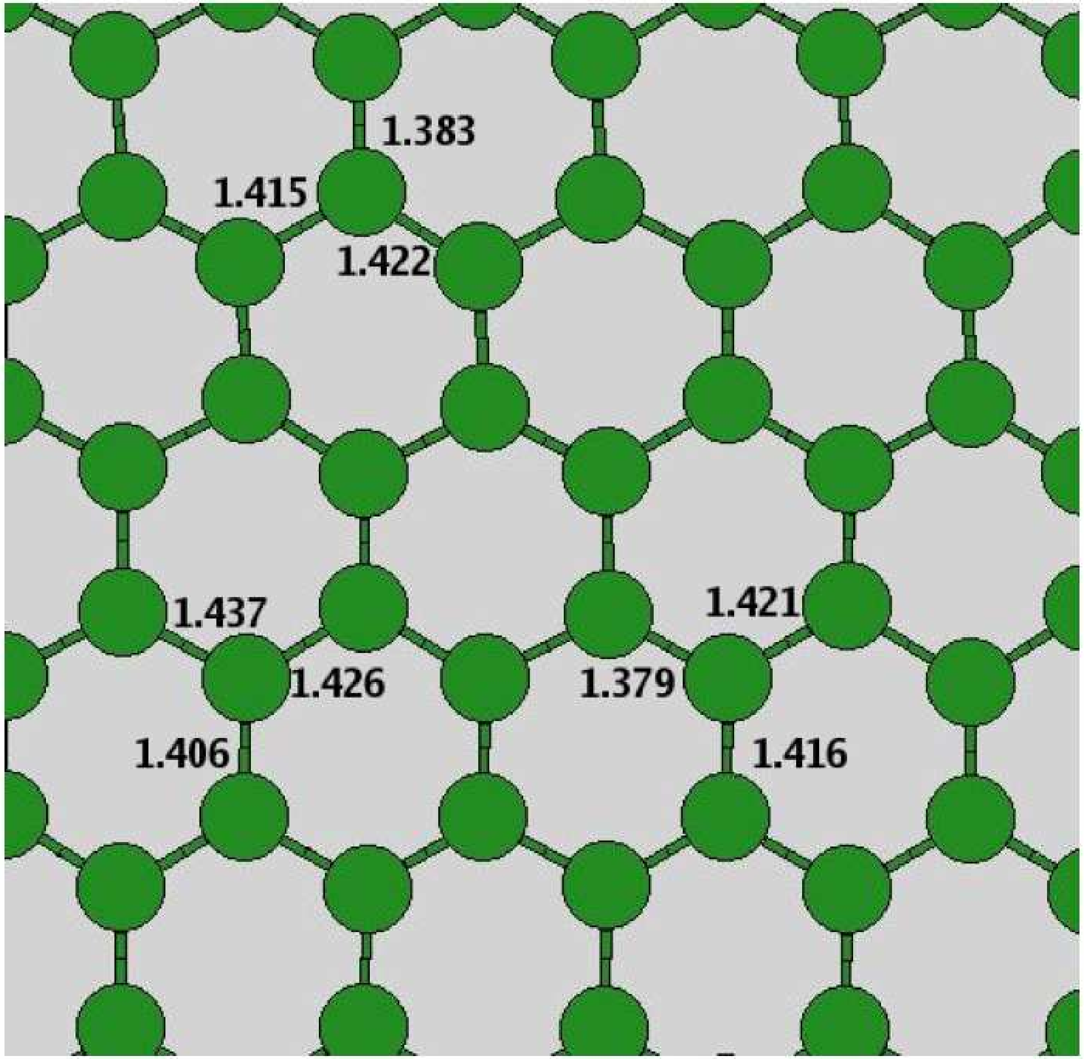


FIG. 5: Radial distribution function for the $N = 8640$ sample at $T = 300$ K and $T = 3500$ K as a function of interatomic distances in Å. The arrows indicate the length of double ($r = 1.31$ Å), conjugated ($r = 1.42$ Å) and single ($r = 1.54$ Å) bonds.

Chemical bonds II



RT: tendency to formation of single and double bonds instead of equivalent conjugated bonds

Bending for "chemical" reasons

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"

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

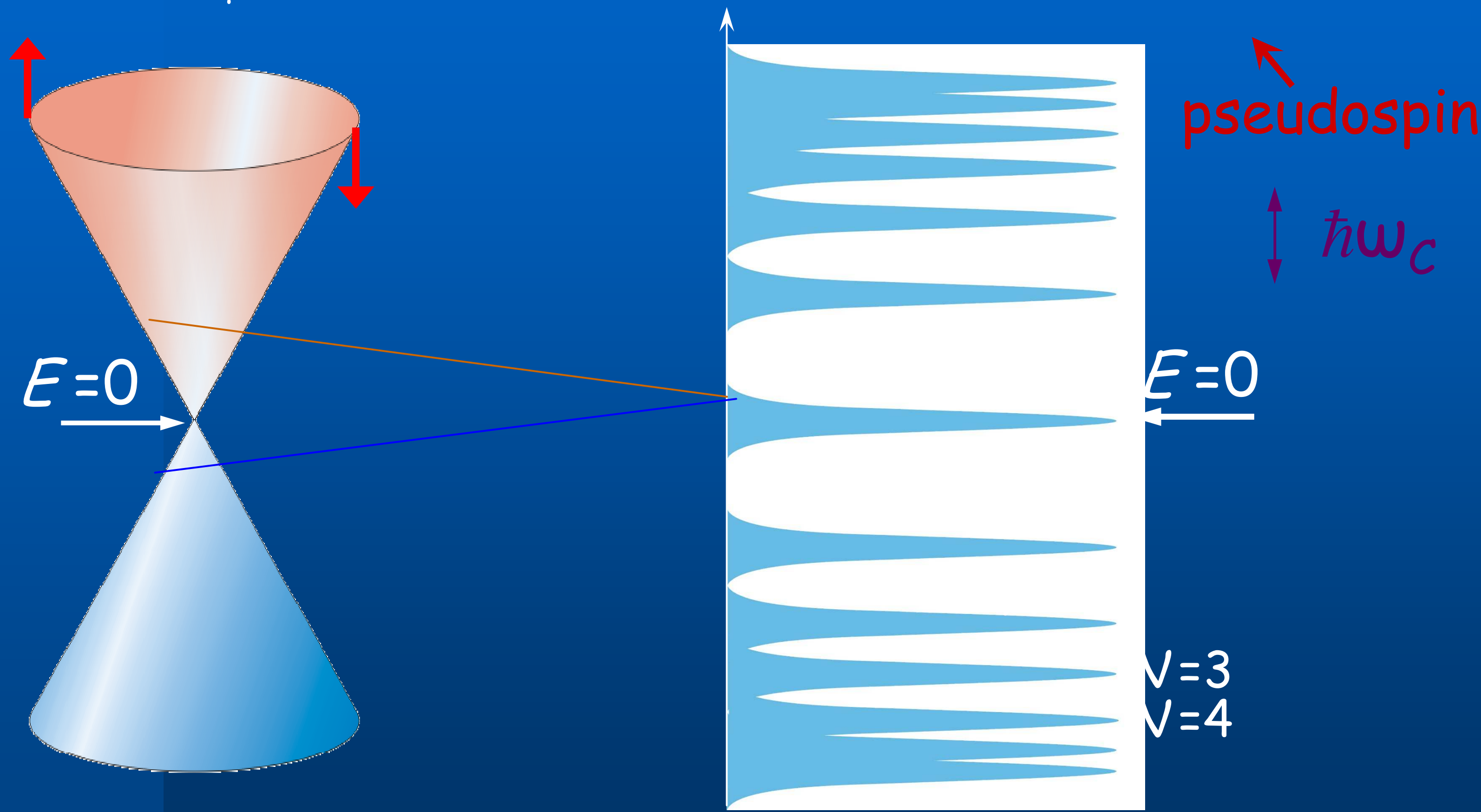
K **and** ***K'*** **points are shifted in opposite directions; Umklapp processes restore time-reversal symmetry**

Suppression of weak localization?

Anomalous Quantum Hall Effect

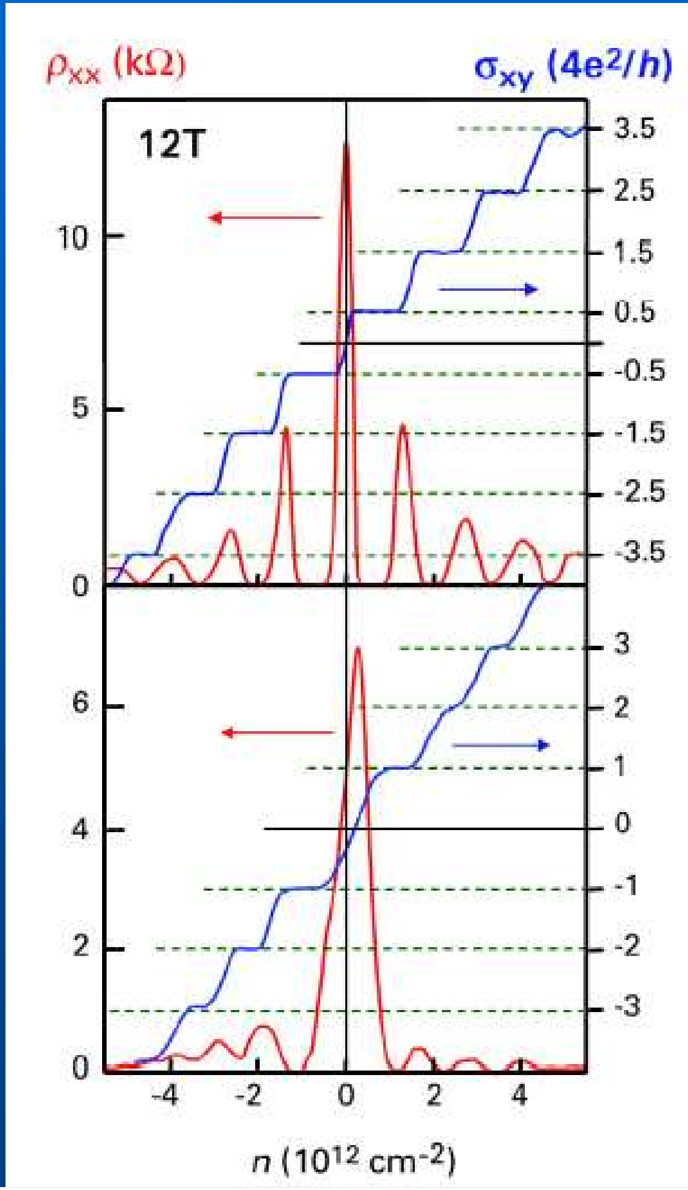
$E = \hbar c_* k$

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



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-*ν* 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)

Consequence: ripples should not broaden zero-energy Landau level

States with zero energy

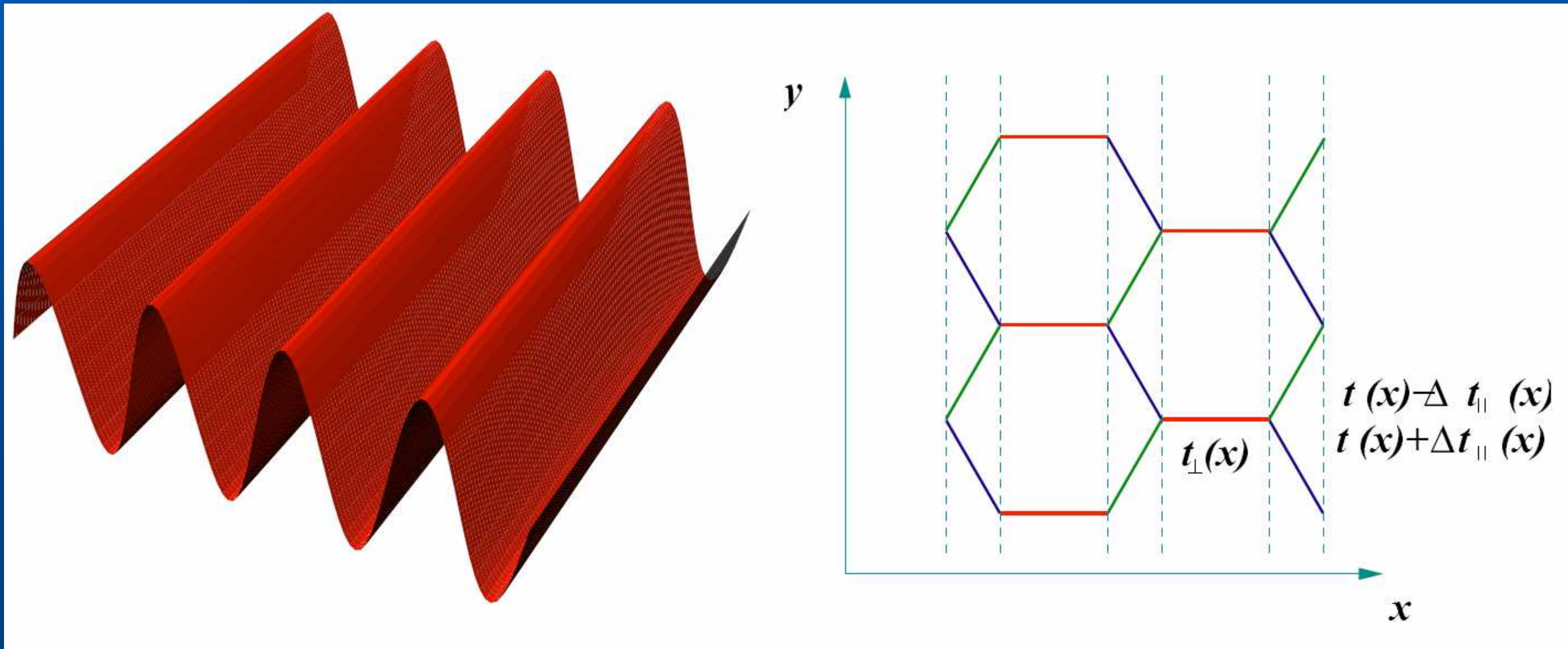
- **Pseudomagnetic fields from the ripples cannot broaden the LL: topological protection**
- **Scalar potential fluctuations broaden zero-enery level in more or less the same way as for other LL's.**

Zero-energy LL should be narrower than all other LL (experiment: J. Giesbers, U. Zeitler, MIK et al, PRL 2007)

Midgap states due to ripples

Guinea, MIK & Vozmediano, PRB 2008

Periodic pseudomagnetic field due to structure modulation



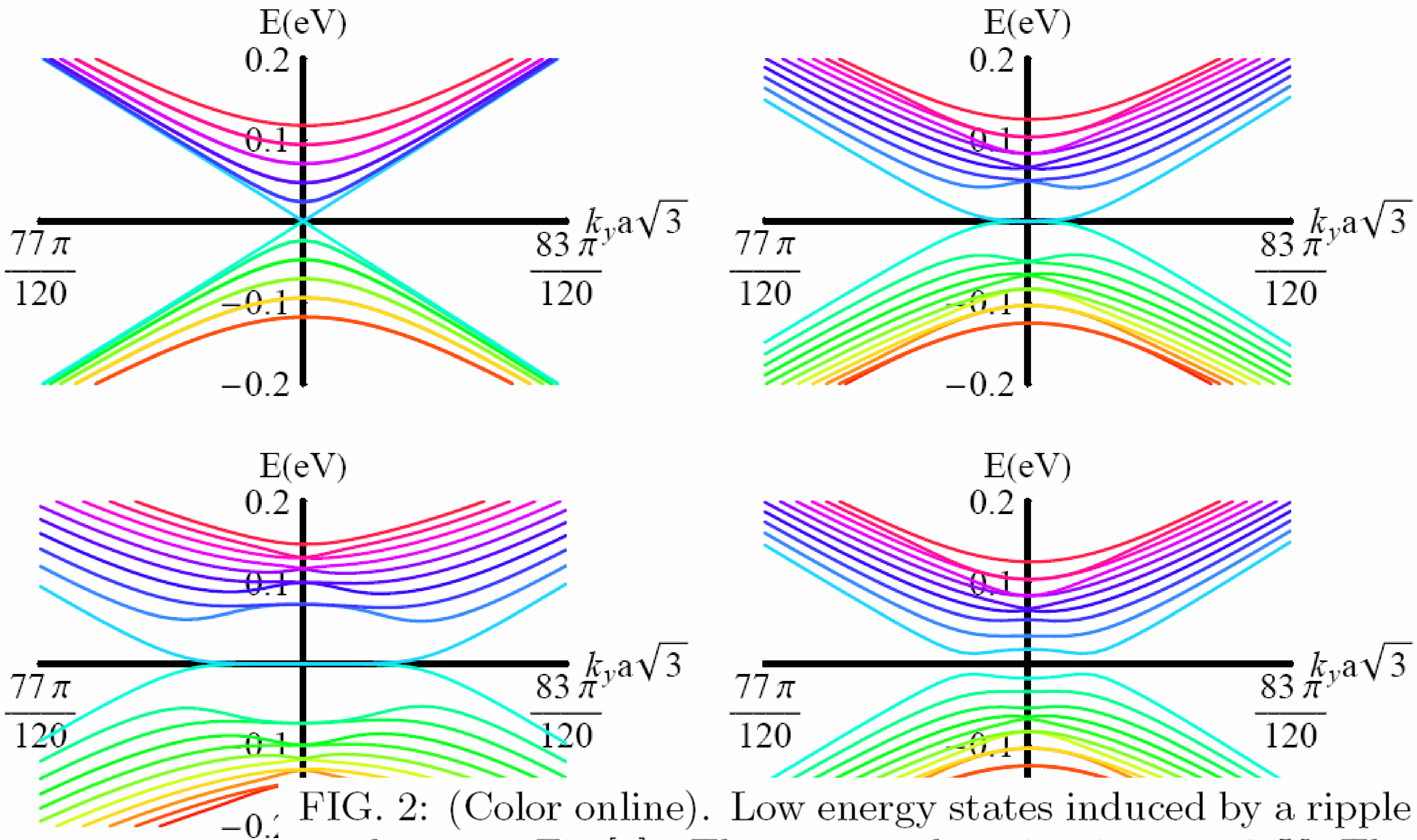


FIG. 2: (Color online). Low energy states induced by a ripple as shown in Fig.[1]. The average hopping is $t_{\|} = 3$eV. The width of the ripple is $1200a = 168$nm. The modulations of the hoppings are: Top left, $\delta t/t = 0$, top right, $\delta t/t = 0.02$, bottom left, $\delta t/t = 0.04$, bottom right, $\delta t/t = 0.02$, and a periodic electrostatic potential of amplitude 0.02eV.

Zero-energy LL is not broadened, in contrast with the others

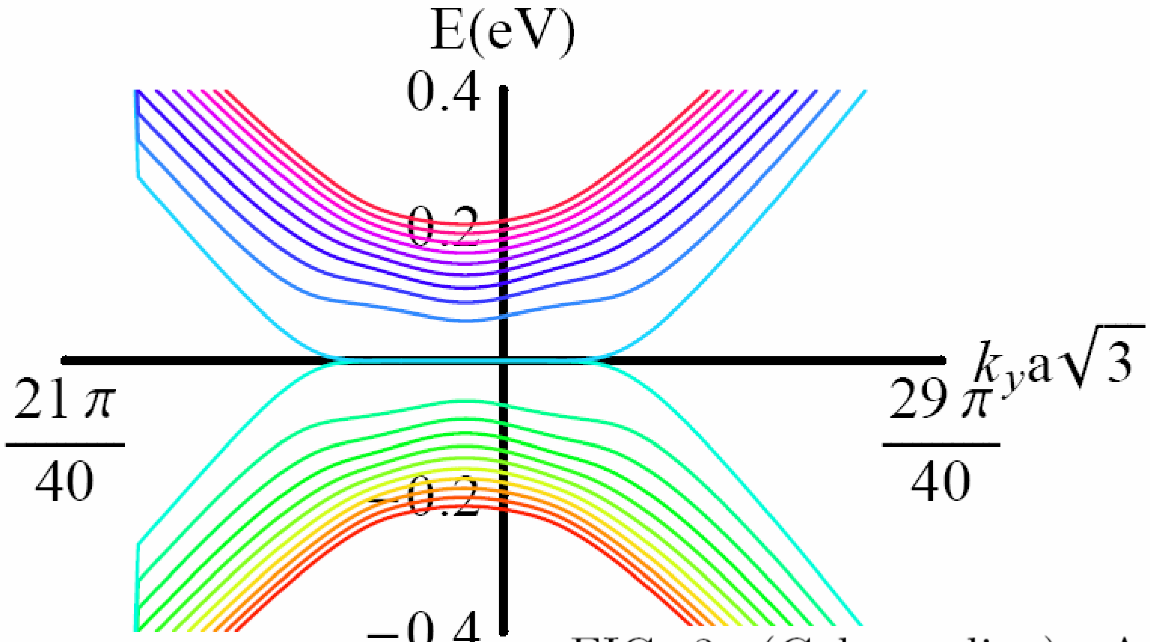
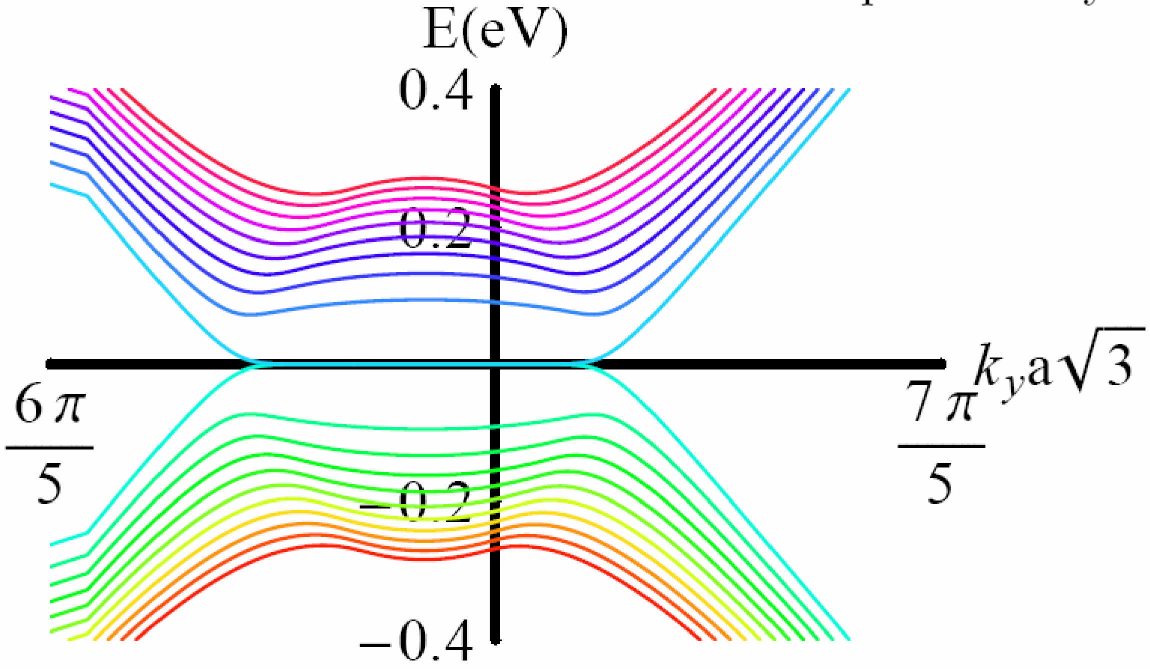


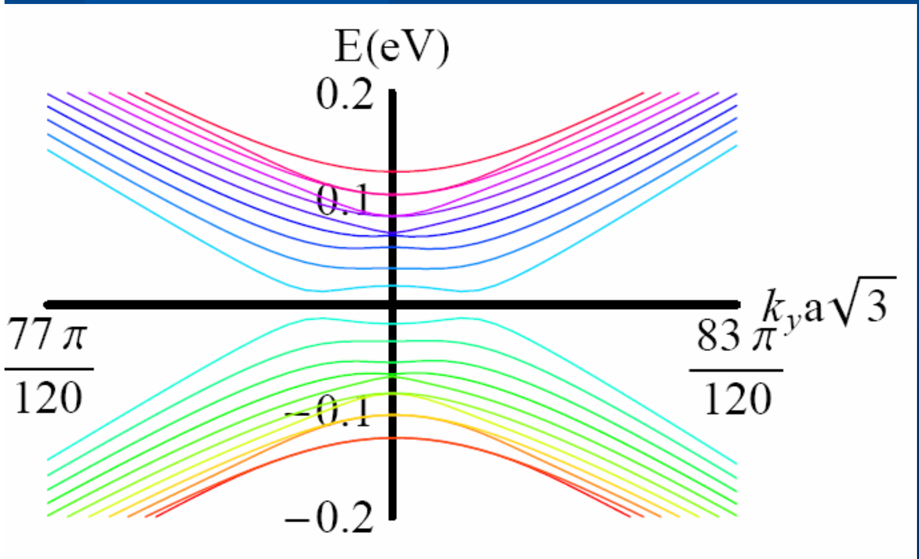
FIG. 3: (Color online). As in Fig.[2], with a magnetic field $B = 10$ T. Top: K valley. Bottom: K' valley.



Mechanism of charge inhomogeneity?

Midgap states (pseudo-Landau levels): infinite compressibility due to δ-functional DOS peak

Charge inhomogeneity opens the gap due to modulation of electrostatic potential



Modulation of NNN hopping (A.Castro Neto): similar effect but probably too small: *t'/t ≈ 1/30.*

Index theorem for bilayer graphene

Low-energy description:
Massive chiral fermions
Berry phase 2π

$$H=\begin{pmatrix} 0 & -(p_x-ip_y)^2/2m \\ -(p_x+ip_y)^2/2m & 0 \end{pmatrix}$$

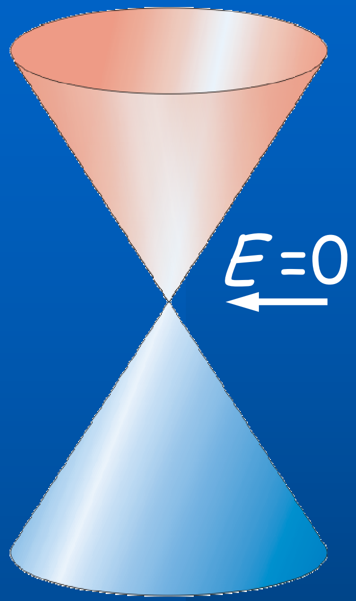
$$m \simeq 0.054 m_e$$

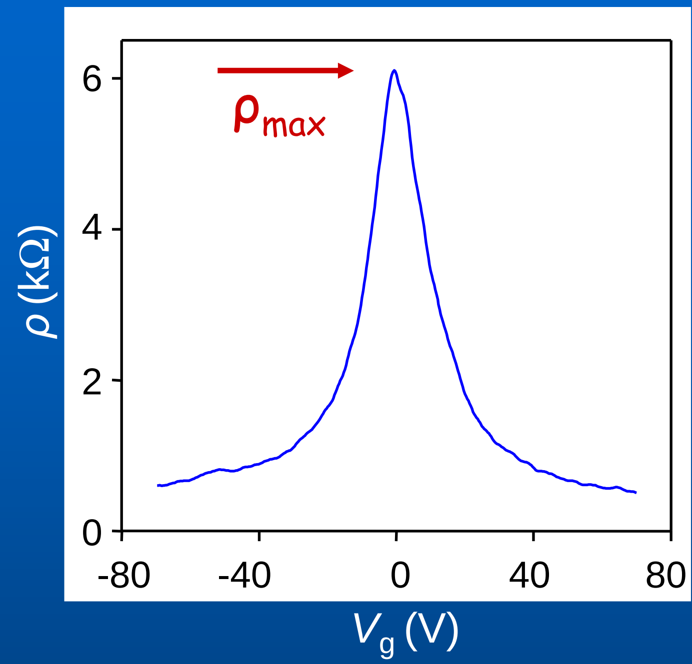
$$N_+ - N_- = 2\phi/\phi_0$$

(MIK and M. Prokhorova, PR B 2008)

Consequences: anomalies of zero-energy Landau level in QHE, mechanism of charge inhomogeneity…

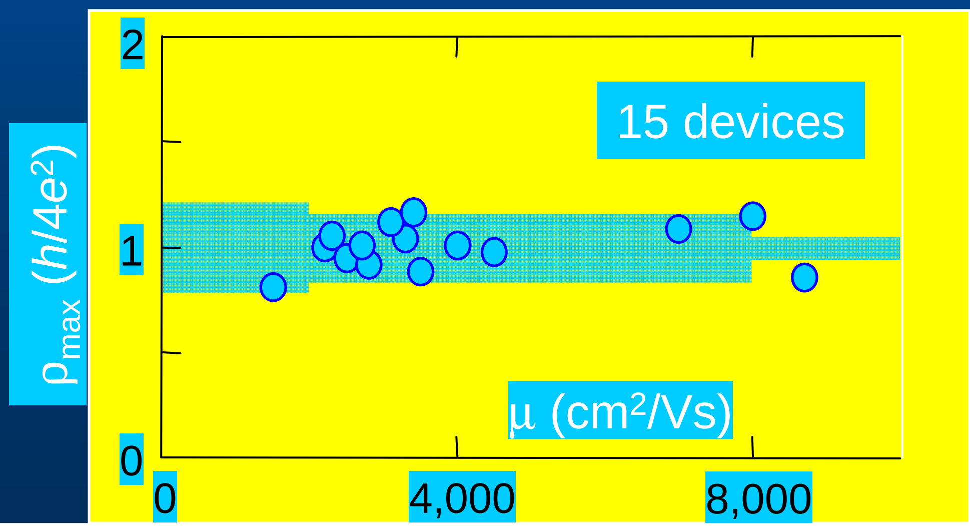
Quantum-Limited Resistivity





no temperature dependence in the peak between 3 and 80K

zero-gap semiconductor



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

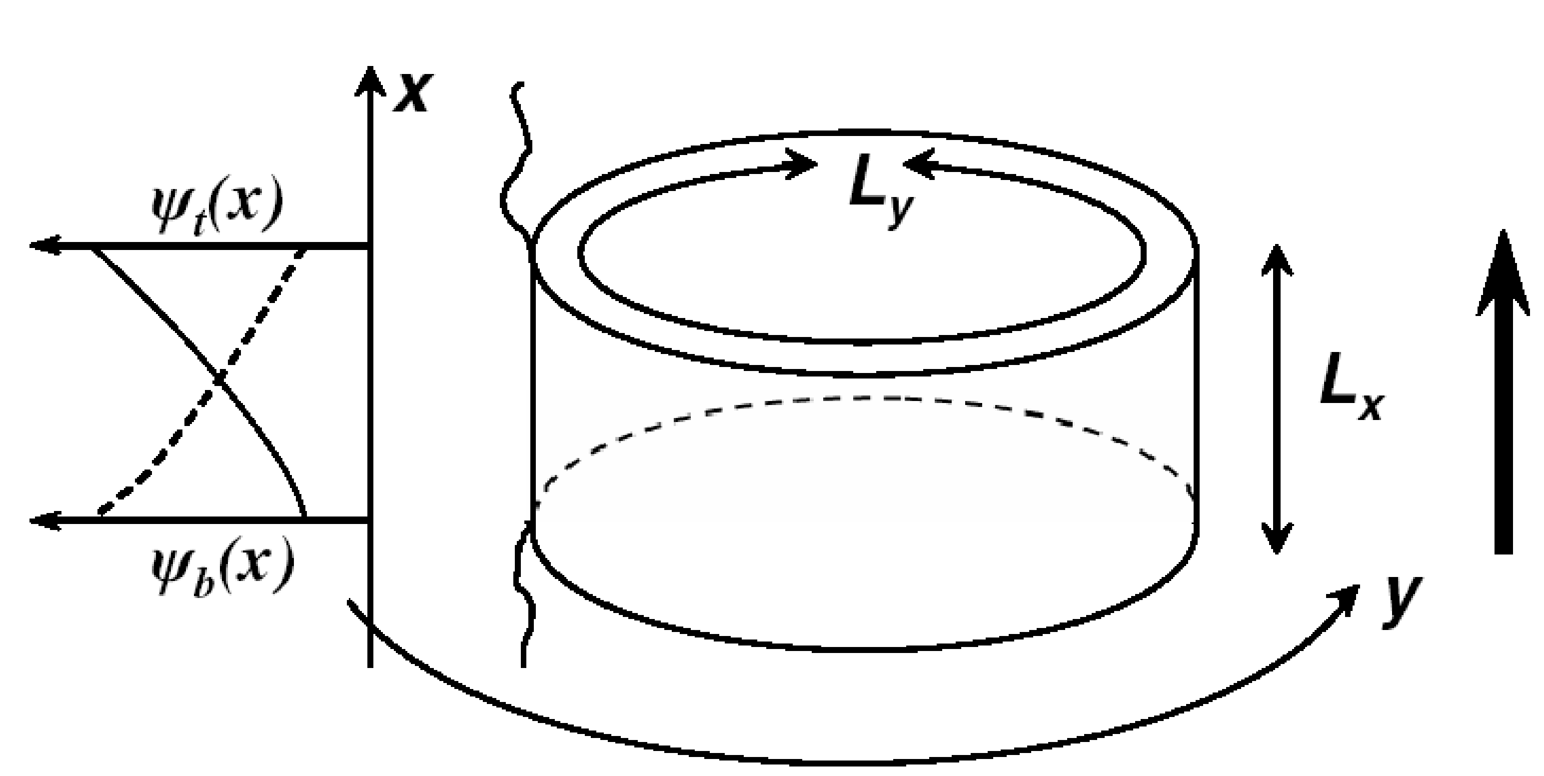
T is the transmission probability matrix

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



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

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

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

$$\sigma\left(\omega\right)=\frac{1}{2A}\int_{0}^{\infty}dte^{i\omega t}\int_{0}^{\beta}d\lambda\left\langle \mathbf{j}\left(t-i\lambda\right)\mathbf{j}\right\rangle$$

Indeterminacy 0•∞ due to Zitterbewegung

Resulting static conductivity of order of e^2/h

Quantum Boltzmann Equation I

Derivation of the Boltzmann kinetic equation with taking into account Zitterbewegung: M. Auslender & MIK, PRB (2007)

General idea of coarse-grained description: Kohn & Luttinger 1957 for normal metals

Method used: Nonequulibrium statistical operator (NSO) approach (Zubarev, Peletminskii…)

One postulates that there is a closed set of equations for some operators (“gross variables”), and this is enough to formulate these equations (some small parameters, e.g., scattering Potential, defect concentration, etc. are necessary)

Quantum Boltzmann Equation II

Starightforward calculations up to the second-order in *V* results in a complicated set of singular integral equations (PR B 76, 235425 (2007))

$$U(\mathbf{r}) = U_0 \Omega \delta(\mathbf{r})$$

(cutoff at a bandwidth is necessary)

Exponentially small energy scale appears, similar to the Kondo problem:

$$\epsilon_{\mathrm{K}} = \epsilon_c e^{-1/2\Phi} = \epsilon_c e^{-\pi\sigma_{\mathrm{B}}}$$

$$\Phi = \frac{c U_0^2 \Omega}{4\pi v^2 \hbar^2}$$

σ_{B} is the Bornian conductivity in units e^2/h

Quantum Boltzmann Equation III

$$\epsilon_c \gg |\mu| \gg \max(\epsilon_K, T)$$

Zittebewegung is negligible, classical BE works!

Zero doping (minimal conductivity regime):

$$\sigma \approx \sigma_B \begin{cases} 1 + \dfrac{\pi^2}{4} + \dfrac{\pi^2}{16}\left(\ln \dfrac{\epsilon_K}{T}\right)^{-1}, & T \ll \epsilon_K \\ 1 + \dfrac{\pi^2}{16}\left(\ln \dfrac{T}{\epsilon_K}\right)^{-1}, & T \gg \epsilon_K \end{cases}$$

$$\frac{\sigma(0)}{\sigma(\infty)} = 1 + \frac{\pi^2}{4}$$

Chiral tunneling and Klein paradox

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

Classical particles: cannot propagate through potential barriers

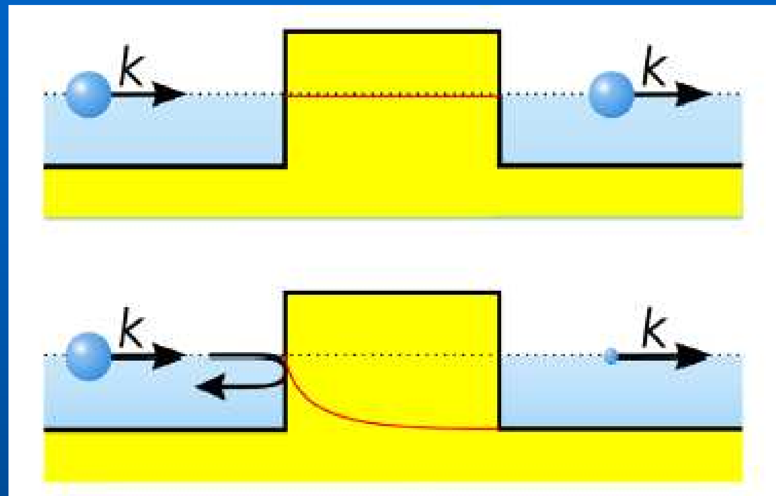
Quantum particles: can propagate (tunneling) but probability decays exponentially with barrier height and width

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

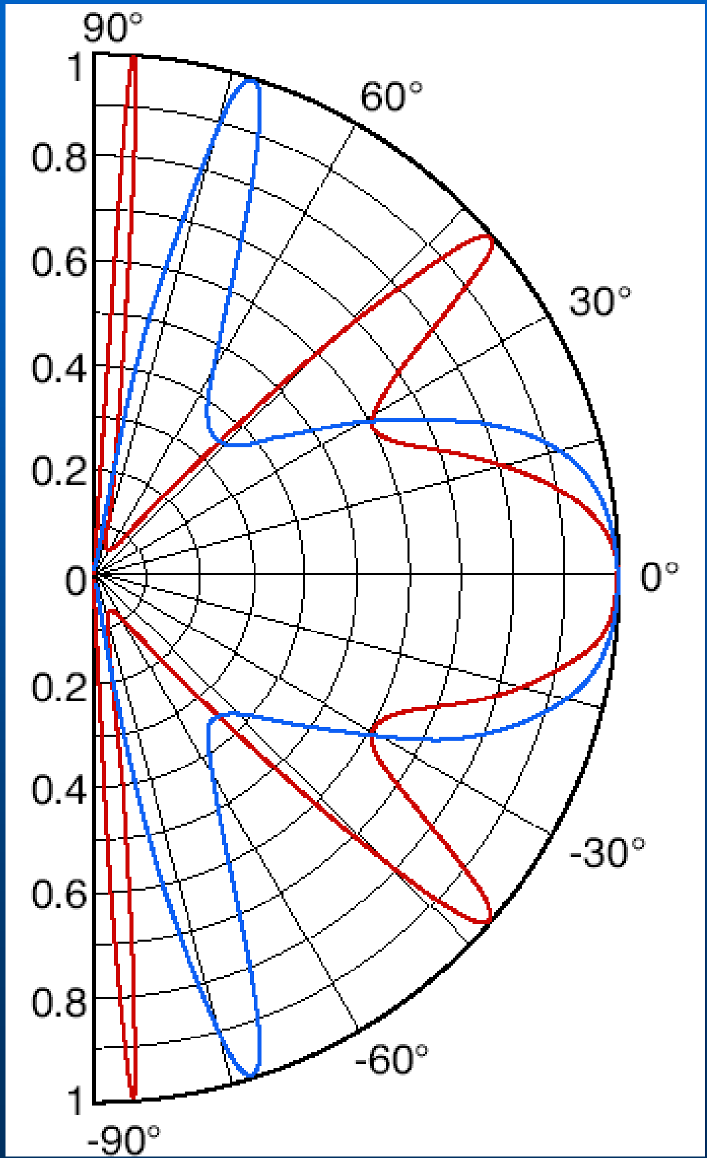
Klein paradox III

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)

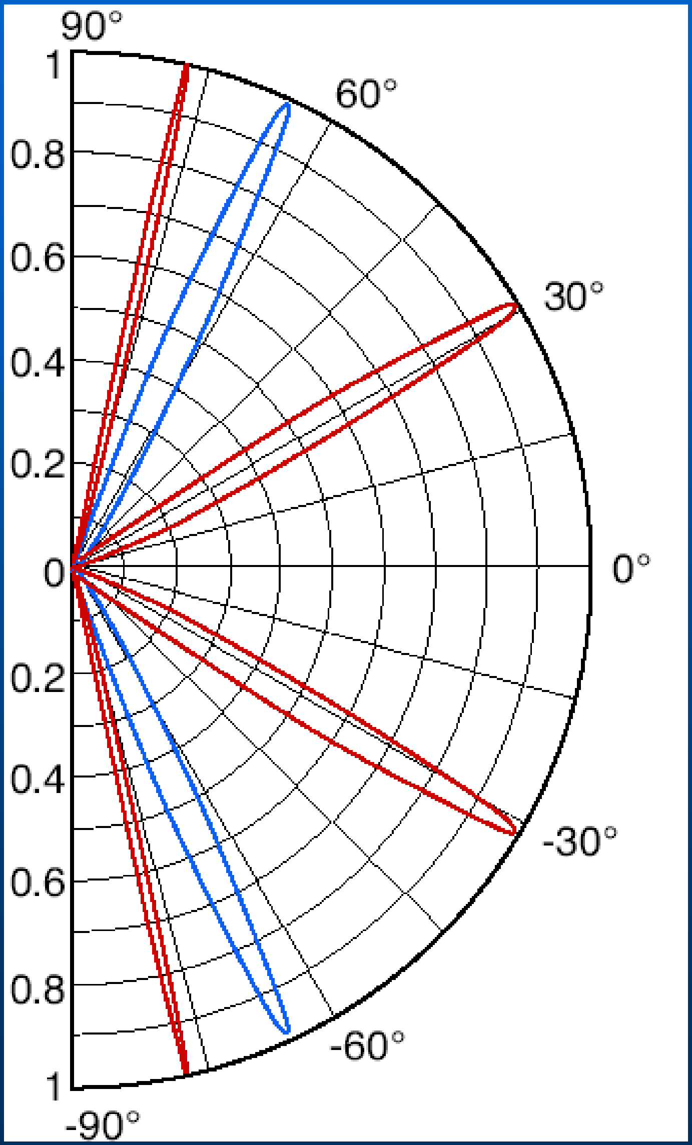


Klein paradox IV

A problem: graphene transistor can hardly be locked!

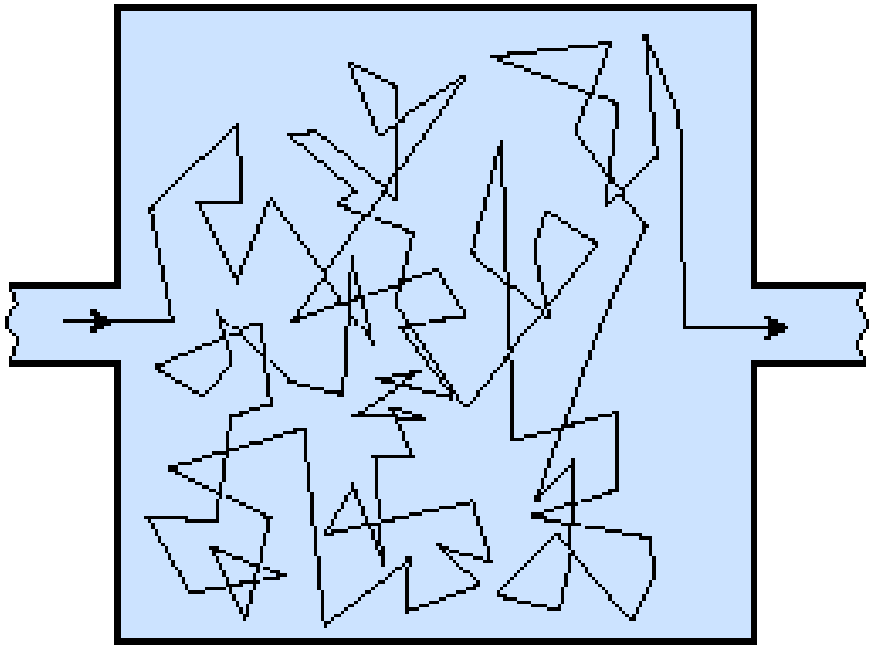
Possible solution: use bilayer graphene: chiral fermions with parabolic spectrum – no analogue in particle physics!

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



Klein paradox and the problem of localization

Back scattering is forbidden for chiral fermions! Magic angle = 0
Nonuniversal magic angle for bilayer exists!



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

Charge impurity in graphene: Vacuum polarization effect

Coulomb potential

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

Dimension analysis: induced charge density

$$n(r) = A\delta(\mathbf{r}) + B/r^2$$

Linear screening theory: constant dielectric function, screening charge focused at the coordinate origin (only first term)

Nonlinear screening

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

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

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

Nonlinear screening – Thomas-Fermi II

Effective impurity charge

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

Inverse linear screening radius

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

$$Q = 2\left(\frac{e^2}{\epsilon \hbar v_F}\right)^2$$

A very strong suppression: tens of times???

General formulation

(A. Shytov, MIK, L. Levitov, PRL 2007)

Thomas-Fermi theory is asymptotically accurate in the large *Z* limit

Perturbatively (small *Z*) logarithmic divergence at large *r* should be absent

Key quantum-relativistic phenomenon: electron fall at the Coulomb centre for $\beta = Ze^2/\hbar v_F \varepsilon > 1/2$ (in 3D case $\beta > 1$).

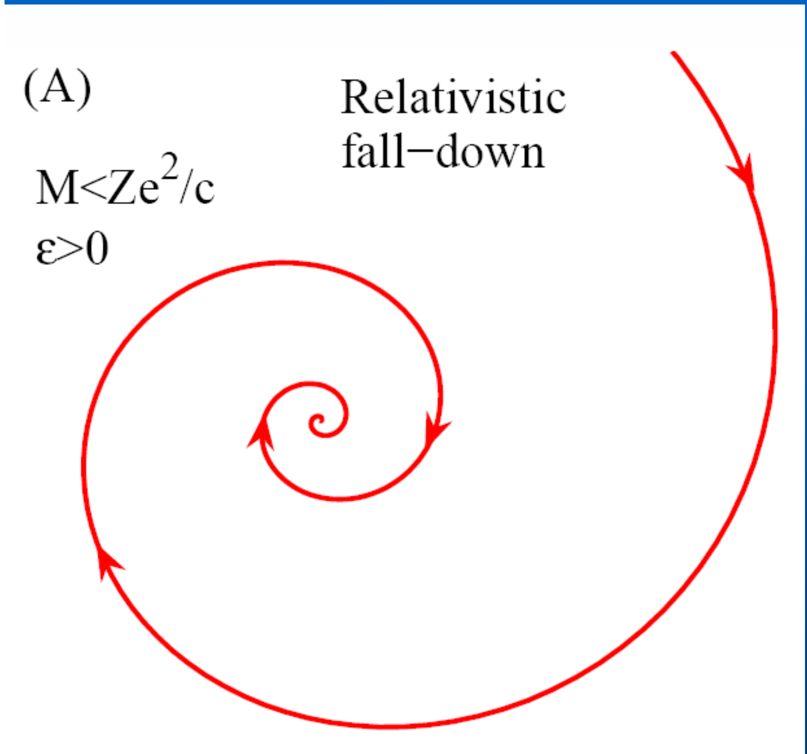
Method:

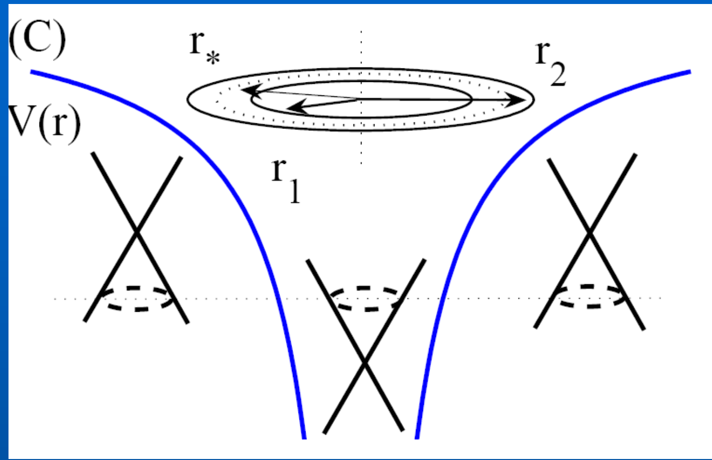
Explicit solution of the Dirac-Kepler problem

Naive arguments: Radius of atom *R*, momentum *ħ/R*. Nonrelativistic case:
$E(R) \sim \hbar^2 / mR^2 - Ze^2/R$
Minimum gives a size of atom.
Relativistic case: $E(R) \sim \hbar c^*/R - Ze^2/R$
Either no bound state or fall on the center.

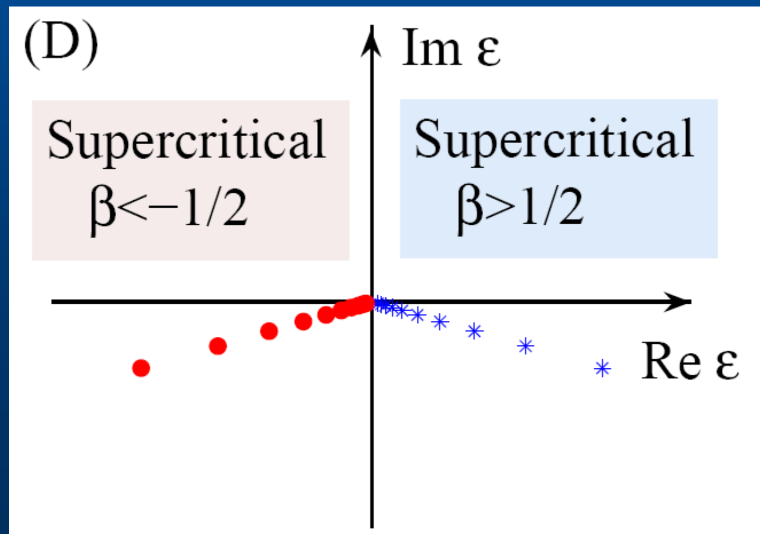
Vacuum reconstruction at $Z > 170$

$\beta > ½$ *Electron fall on the center*





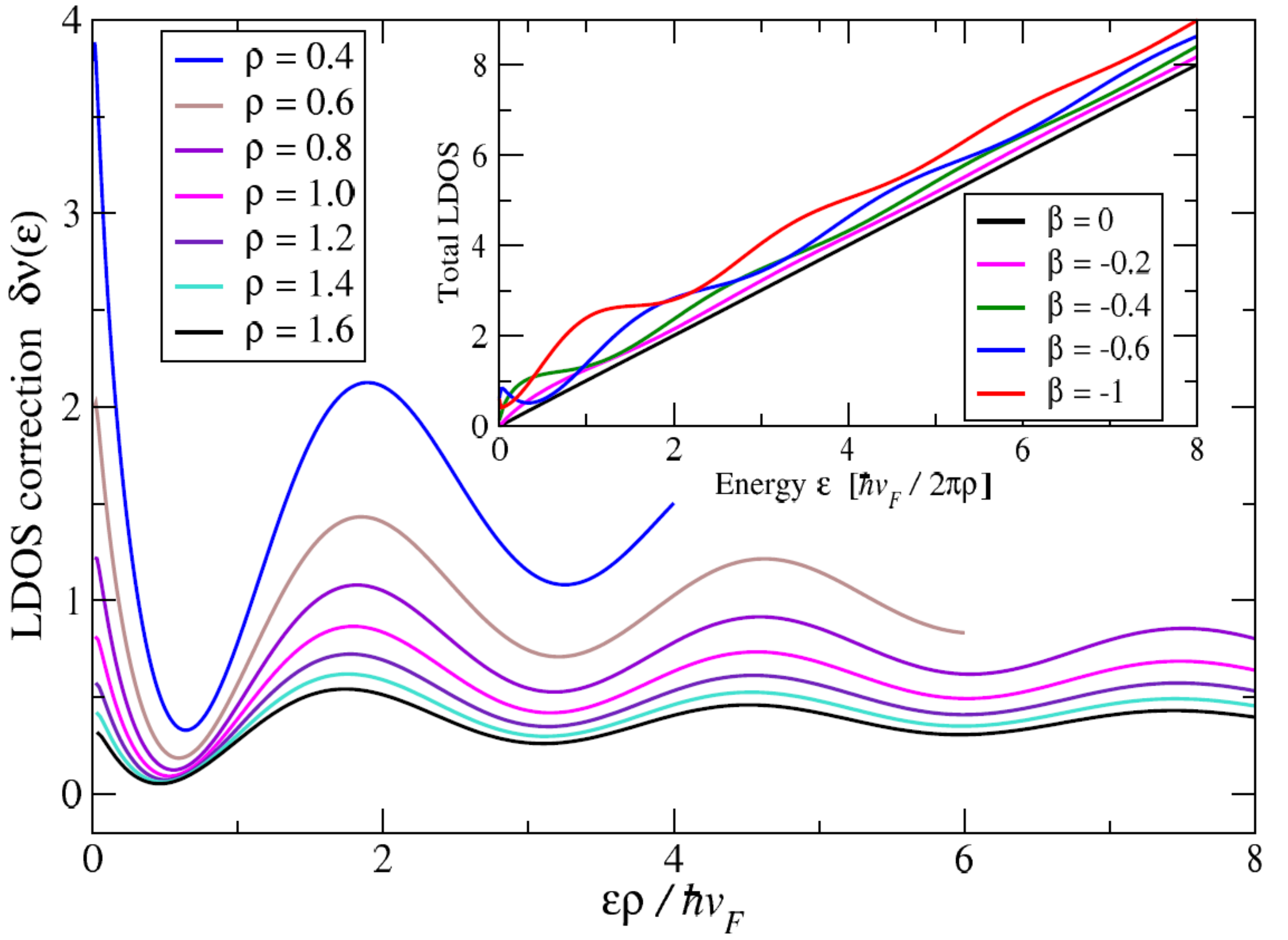
Klein tunneling



Quasi-local states

Supercritical charge

Interference of scattered wave and wave described electron fall to the centre leads to oscillations of electron density



β = 0.6

Inset: oscillations for different charges

Supercritical charge II

$$n_{\mathrm{pol}}(\rho) = -\frac{N \,\mathrm{sign}\,\beta}{2\pi^2\rho^2} \sum_{|m+\frac{1}{2}|<|\beta|} \sqrt{\beta^2 - \left(m+\frac{1}{2}\right)^2}$$

N = 4 (two valleys, two spins)

Large *β*: replacing the sum by an integral recover the Thomas-Fermi result

RG analysis: all supercritical charge is screened to *β* = ½ with a finite screening radius (similar to black hole horizon)

Conclusions and final remarks

- **Relativistic effects are of crucial importance for graphene physics and applications (minimal conductivity, absence of localization, carbon transistors…)**
- **Specific of 2D systems: ripples**
- **Exotic phenomena in everyday's life (e.g., Klein paradox, vacuum reconstruction)**
- **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 "nullification")**

Collaboration

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Discussions

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