# Size quantization of the Dirac fermions in graphene

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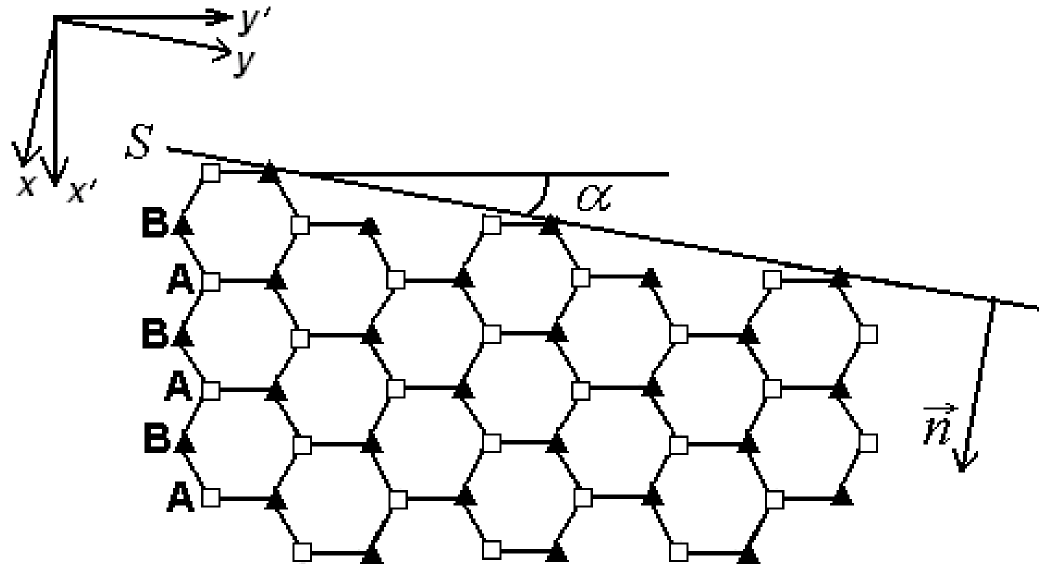
# Introduction: Edge States (ESs) and Boundary Conditions (BCs)

- **The Tamm (**here: **the Tamm-Dirac) problem: spectra of edge states w/o magnetic field**
- **Approaches:**

  **1) microscopic models (tight-binding approx. - TBA),**

  **2) effective-mass approximation (EMA)**
- **For EMA: problem of BCs for envelope functions on edge of the sample**
- **Approach (**used here**): phenomenological BCs** (the Hermiticity and time-reversal symmetry)

# What known about BCs and ESs in graphene




## Nearest neighbour tight-binding approximation (TBA)

Nakada, Fujita et al (1996), Brey, Fertig (2006)

**Results**: simple BCs
ESs for zigzag edge: dispersionless Tamm band
ESs for armchair edge: no Tamm states

## Next nearest neighbours TBA

Peres et al (2006), Sasaki et al (2006)

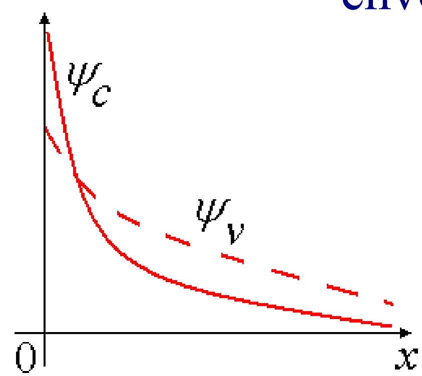
**Result**: finite dispersion of Tamm band at zigzag edge

## "Infinite-mass" BCs : Berry, Mondragon (1987)

***Result***: very simple BC, no ESs.

# Introduction: Envelope Functions and Boundary Problem

$$\varphi_{micro} = \sum_n u_{n0}\left(\vec{r}\right)\psi_n\left(\vec{r}\right)$$



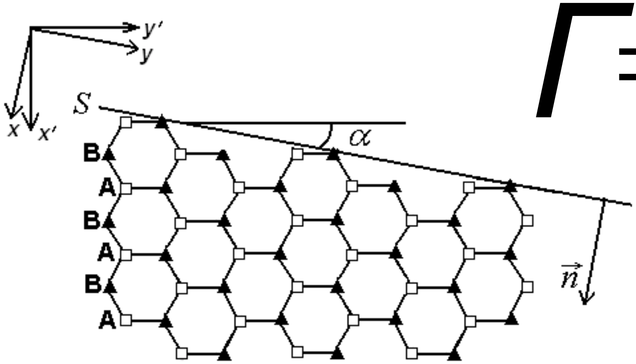

envelope functions column

$$\varphi_{micro} \to \begin{pmatrix} \psi_1\left(\vec{r}\right) \\ \vdots \\ \psi_n\left(\vec{r}\right) \\ \vdots \end{pmatrix}$$

$$\begin{cases} H\psi = E\psi \\ \Gamma\psi\,|_S = 0 \end{cases}$$

$H$ - matrix effective-mass Hamiltonian

$\Gamma$ - a boundary operator.



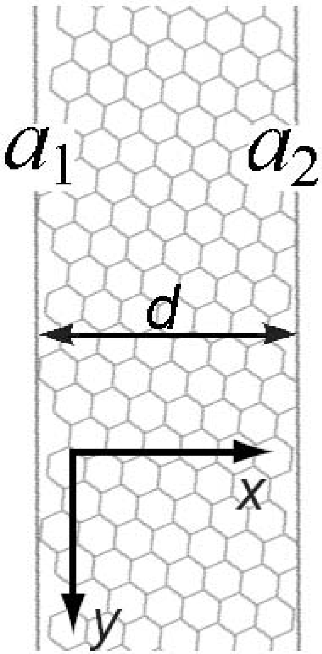

$$\Gamma = ?$$

**V. Volkov, T. Pinsker (1981)**
**M. Berry, R. Mondragon (1987)**
**E. McCann, V. Fal'ko (2004)**
**A. Akhmerov, C. Beenakker (2008)**
**V. Volkov, I. Zagorodnev (2009)**

# <u>The aims of the work:</u>

- to investigate the size quantization problem in graphene using the derived boundary conditions for the Dirac Eq.
- to find electron spectra in <u>graphene nanoribbon</u> taking into account the edge states (”the Tamm-Dirac states”)
- to find spectra of electron states in <u>graphene antidot</u>
- to consider the <u>Aharonov-Bohm effect in graphene antidot</u>
- to discuss an experiment

# Graphene nanoribbon: METHOD




## The Weyl-Dirac equations:

$$\tau\, c\, \boldsymbol{\sigma}\mathbf{p}\, \Psi_\tau = E_\tau \Psi_\tau,$$

Graphene has 2 valleys numbered by τ=±1,
**σ** = ($\sigma_x$,$\sigma_y$) are the Pauli matrices.

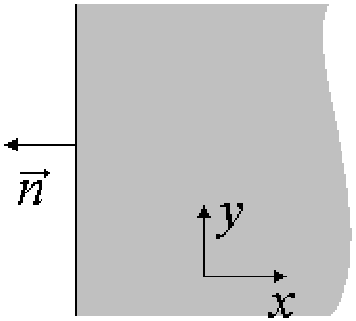
$$\Psi_\tau = \begin{pmatrix} \Psi_{\tau 1} \\ \Psi_{\tau 2} \end{pmatrix}$$

## Boundary conditions*:

$$(\psi_{\tau 1} + i a^{\tau} e^{-i\alpha} \psi_{\tau 2})|_{\Gamma} = 0,$$

$a$ is a real edge parameter

$$\vec{n} = (\cos\alpha, \sin\alpha)$$

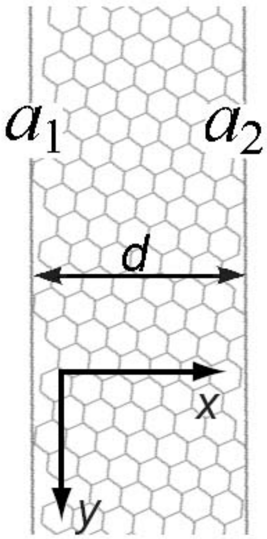


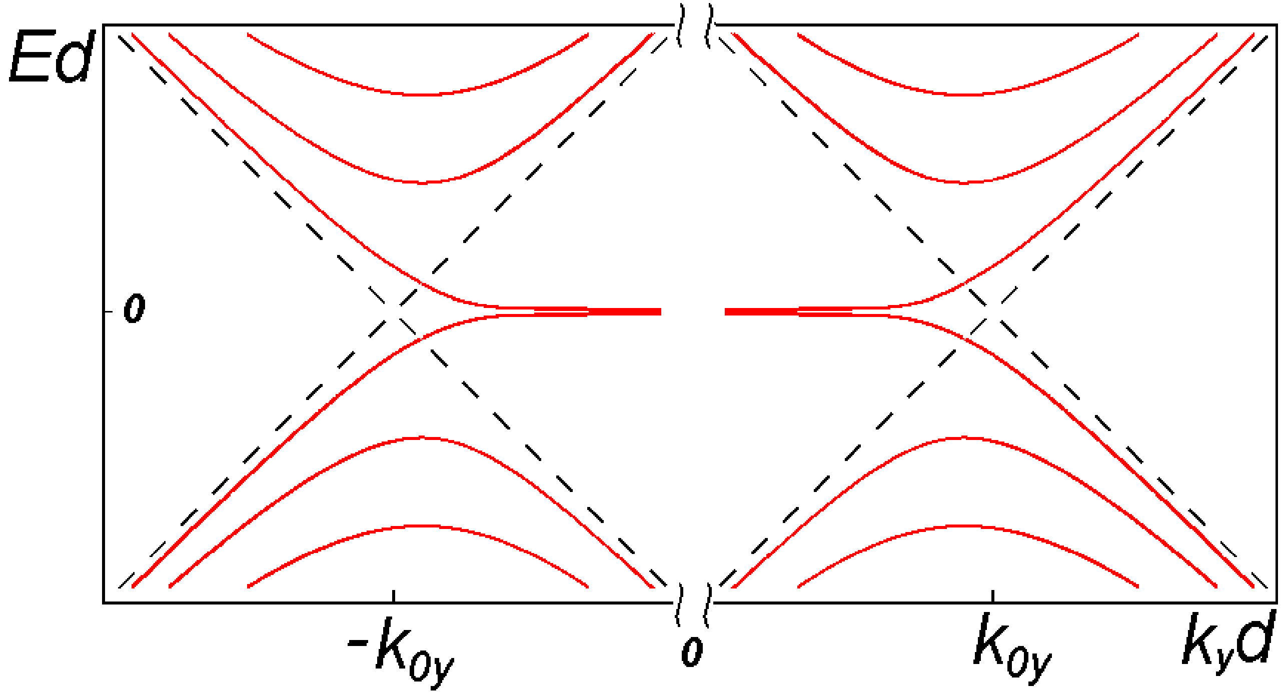

## Dispersion equation:

$$(1- a_1 \cdot a_2)E+(a_2-a_1)k_y - (a_1+a_2)k_x \text{ ctg } k_x d = 0$$

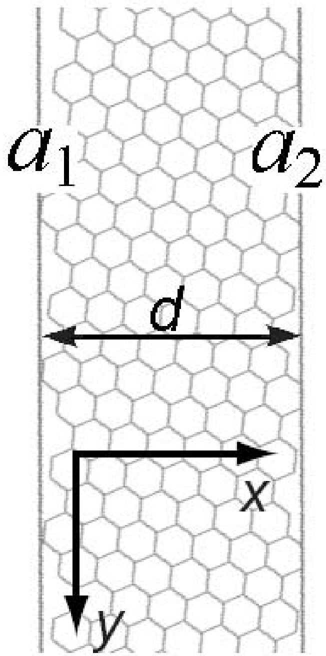
*В. Волков, И. Загороднев *ФНТ* **35**, 5 (2009)
V. Volkov, I. Zagorodnev *J. Phys.: Conf. Ser.* **193**, 012113 (2009)

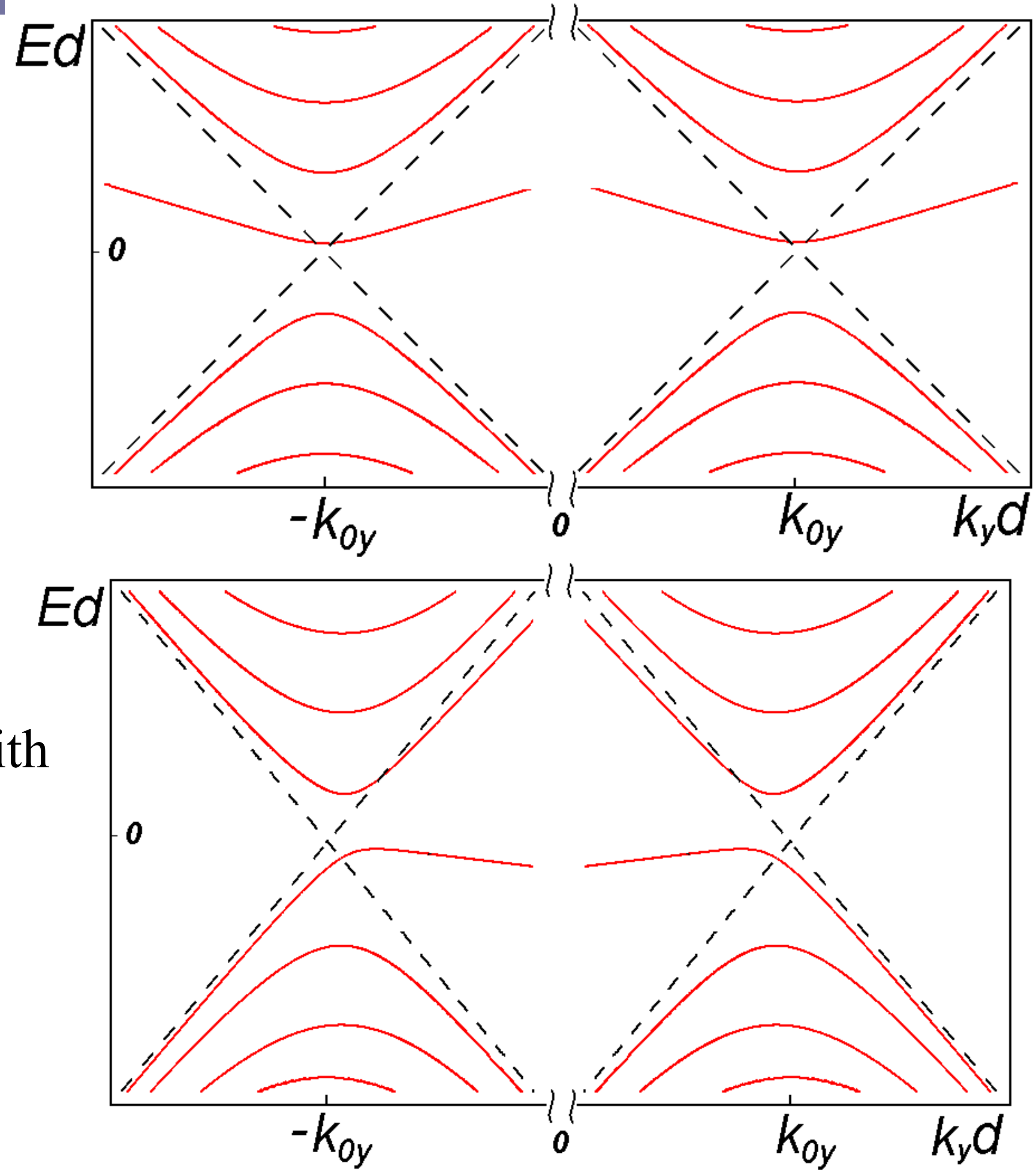
# Graphene nanoribbon: zigzag in TBA




1D subbands $E(k_y)$ for the nanoribbon with zigzag-like model edges ($a_1 = 1/a_2 = 0$). Dotted line: border of volume spectrum, $|E| = c|k_y|$.



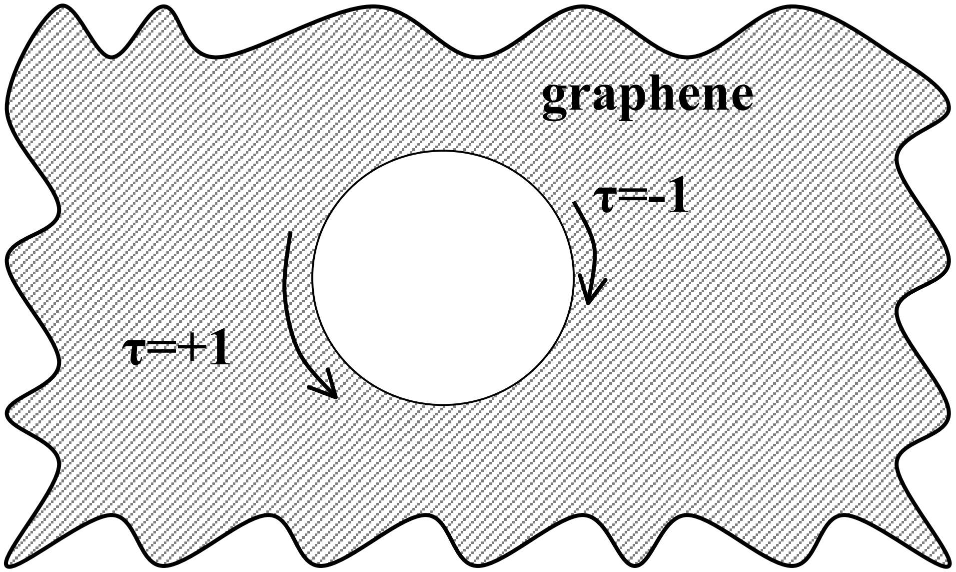




Subbands $E(k_y)$ for graphene nanoribbon with
(a) symmetrical edges
$(a_1 = a_2 = 0.15)$
and
(b) very asymmetrical
$(a_1 = 0.6,\ a_2 = 20)$ edges.

# Graphene antidot as a quantum object

Consider graphene antidot of radius $R_0$. The edge states from different valleys ($\tau = \pm 1$) are occupied by electrons rotating clockwise or counter-clockwise around the antidot. The energies and lifetimes of these states ($\hbar / \mathrm{Im} E_l$ ) are quantized.

$$E_l = \mathrm{Re} E_l + i \, \mathrm{Im} E_l$$




$$\boldsymbol{E_l} R_0/2c = \tau \left(a^\tau l - i \pi a^\tau \left[(a^\tau l)^l / \Gamma(l)\right]^2\right)$$

$l$=1,2,3… - orbital angular momentum, $0 < \tau a^\tau << |l|$,

$c$ – the Fermi velocity, $\Gamma$ – the gamma-function, $a$ – an edge parameter

# The Tamm-Dirac states (see Appendix) in massless limit : $2mc^2 \to 0$

$$H_{Dirac} = \begin{pmatrix} \vec{\sigma}\vec{p} & mc^2 \\ mc^2 & -\vec{\sigma}\vec{p} \end{pmatrix} \to \begin{pmatrix} H_w & 0 \\ 0 & -H_w \end{pmatrix}$$

**2x2 Weyl:** $H_w = \vec{\sigma}\vec{p}$

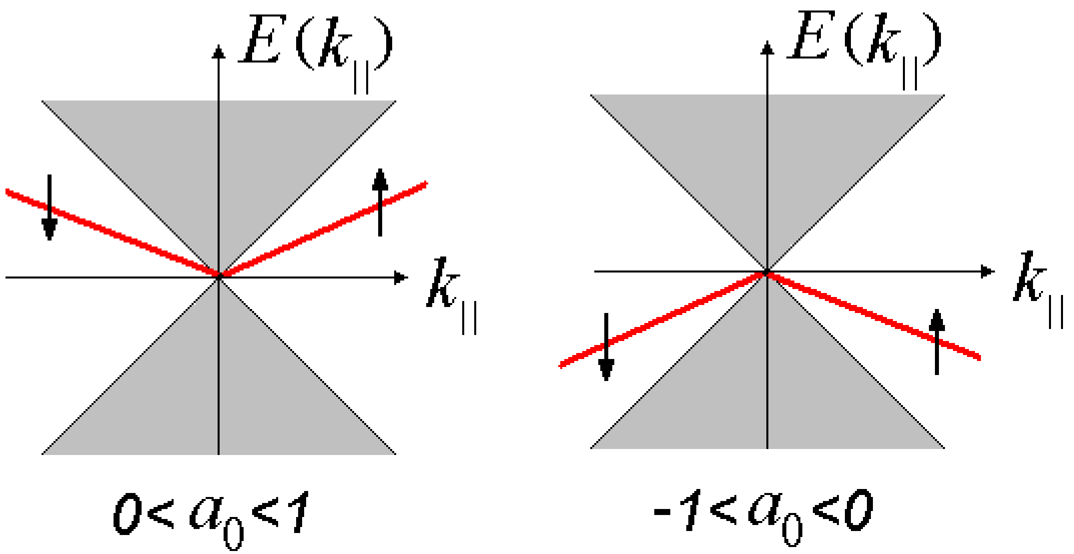
**Boundary conditions:**

$$\left(\psi_c + ie^{ia_0\vec{\sigma}\vec{n}}\psi_v\right)\Big|_S = 0$$

$$E = \frac{2a_0}{a_0^2+1}k_y,$$

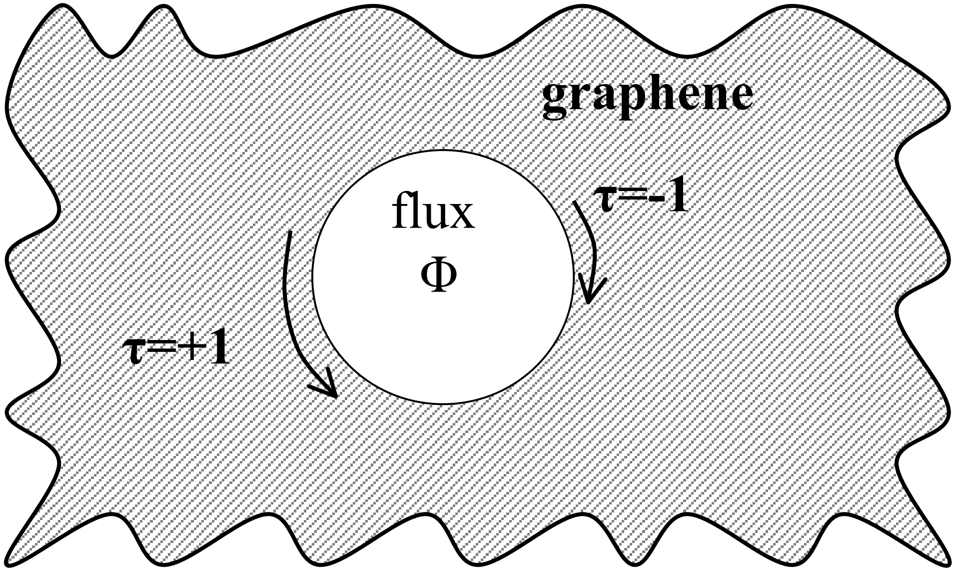
$$where\ k_y\left(1-a_0^2\right) > 0$$

**Tamm-Dirac spectra:**




For the antidot $R_0$ in quasiclassics: $k_y = n/R_0$

# Aharonov-Bohm effect in graphene antidot



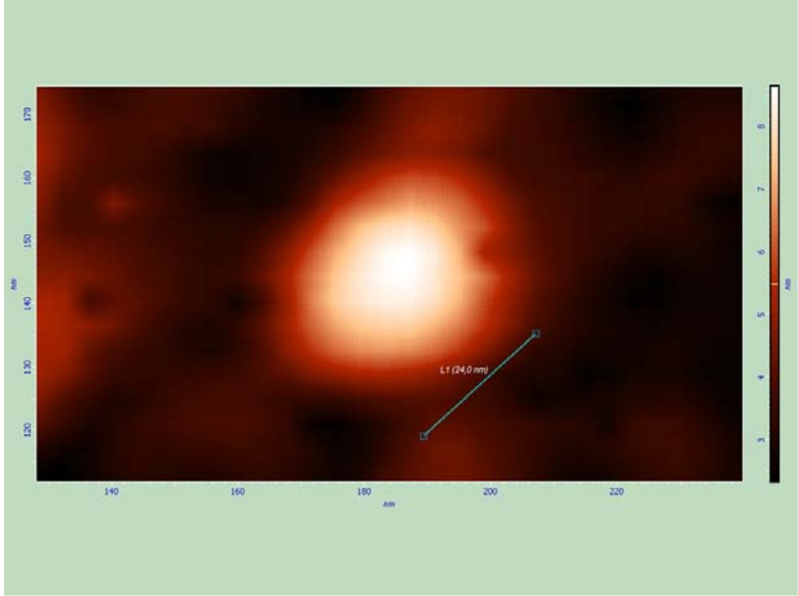

$$\boldsymbol{E_l}\, R_0/2c \approx \tau\, a^{\tau}\, L$$

$L = l + \Phi/\Phi_0$, $l$=1,2,3…, $\Phi = \pi B R_0^{\,2}$, $0 < \tau\, a^{\tau} << 1$,
$c$ – the Fermi velocity, $a$ – an edge parameter, $\Phi/\Phi_0$– the number of magnetic flux quanta through the antidot.

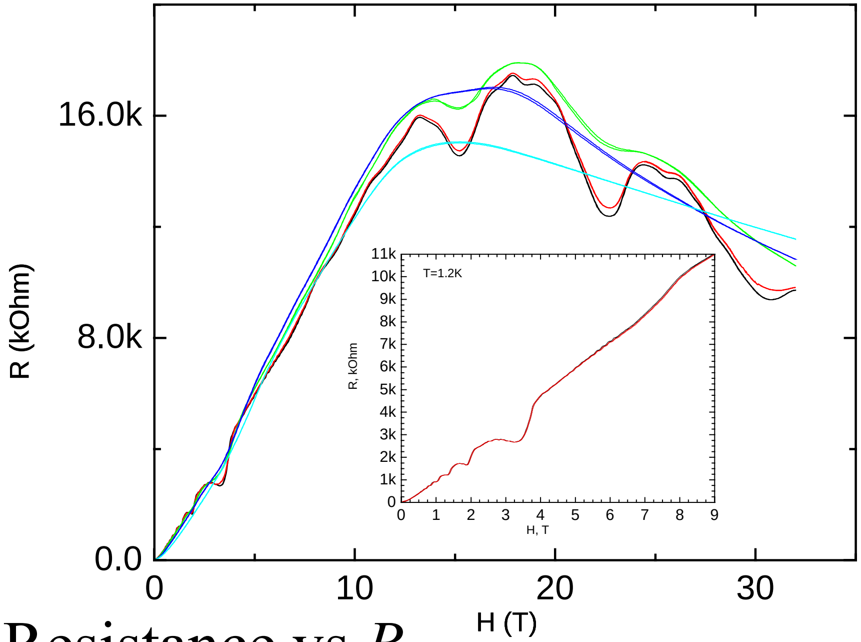
*B*-periodic resistance oscillations in ultrathin graphite crystals with columnar defects (nanoholes) were observed in magnetic field *B*:

***Aharonov-Bohm effect ?***

Yu.I. Latyshev, A.Yu. Latyshev, A.P. Orlov, A.A. Shchekin, V.A. Bykov, P. Monceau, K. van der Beck, M. Kontsikovskii, I. Monnet. JETP Letters, **90**, 526 (2009)



AFM image of a nanohole




Resistance vs *B*,

T= 1.2 - 32 K, c = $10^9$ def/см$^2$.

# RESULTS

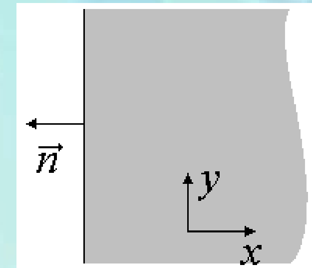
- Analytical theory of energetic structure of **graphene nanoribbon** is proposed taking into account size quantization and edge states. We solve the Weyl-Dirac equation with boundary conditions that was derived by authors earlier. The resulting spectrum depends on two boundary parameters each one characterize one of the boundaries of a nanoribbon. The value of these parameters can be found from comparison with the results obtained in tight-binding or ab intio calculations.
- The edge states around an **antidot** are quantized and form a quasi-equidistant ladder of quasi-discrete states. Accordingly **the graphene antidot is a quantum object.** This unique feature essentially differs graphene from "non-relativistic" systems like GaAs or Si, where electrons are not localized by an antidot. In moderate magnetic field the energies of electrons rotating around the antidot undergo B-periodic oscillations of the Aharonov-Bohm type.

# Appendix: **Tamm states in Dirac band model**

$$\widehat{H}_{kp} = \begin{pmatrix} mc^{*2} & c^{*}\vec{\sigma}\vec{p} \\ c^{*}\vec{\sigma}\vec{p} & -mc^{*2} \end{pmatrix} \qquad \psi = \begin{pmatrix} \psi_c \\ \psi_v \end{pmatrix}$$

$\psi_c = \begin{pmatrix} \psi_{c1} \\ \psi_{c2} \end{pmatrix}$ c-spinor

$\psi_v = \begin{pmatrix} \psi_{v1} \\ \psi_{v2} \end{pmatrix}$ v- spinor




$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

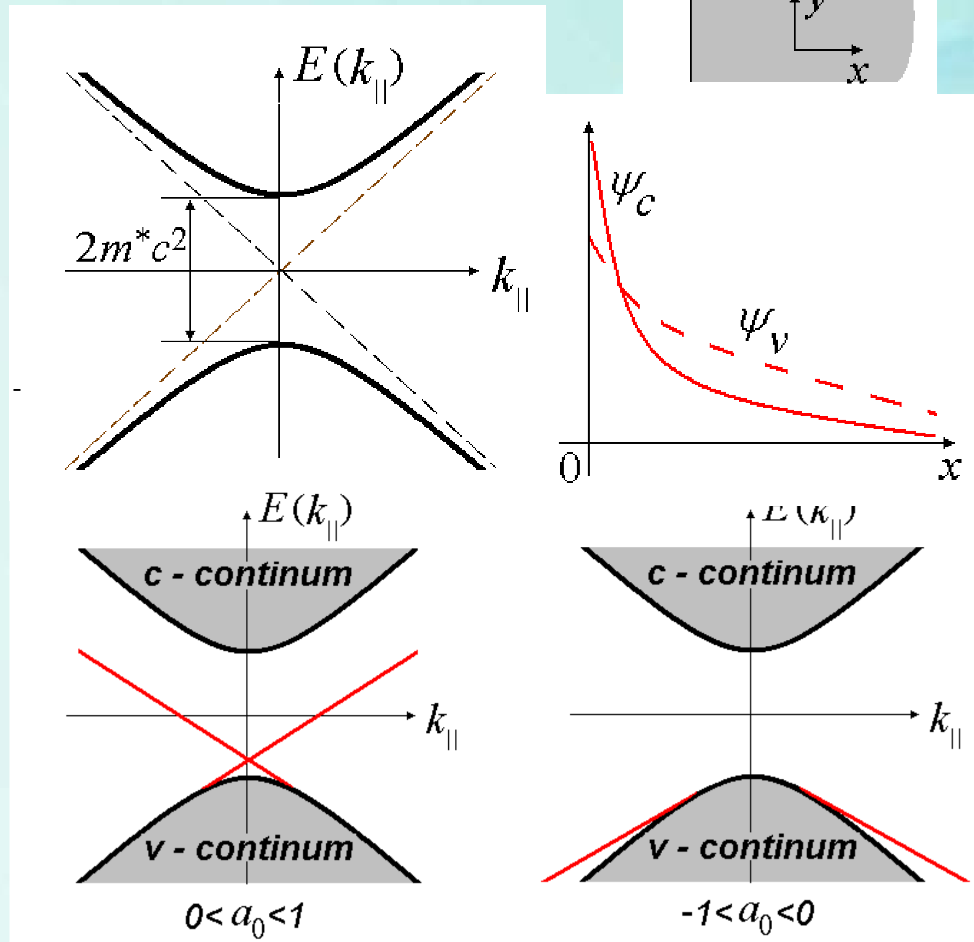
$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\hat{T} = i\begin{pmatrix} \sigma_2 & 0 \\ 0 & \sigma_2 \end{pmatrix}\widehat{K_0}$$

$\widehat{K_0}$ - complex conjugate

Tamm spectra depend on single boundary parameter $a_0$

$$\begin{cases} \widehat{H}^{+} = \widehat{H} \\ \hat{T}\hat{\Gamma}\hat{T}^{-1} = \hat{\Gamma} \end{cases} \Rightarrow \left(\psi_c + a_0\vec{\sigma}\vec{n}\psi_v\right)\Big|_S = 0$$




В. Волков, Т. Пинскер *ФТТ* **23,** 1756 (1981)

[V. Volkov, T. Pinsker *Sov. Phys. Solid State* **23,** 1022 (1981)]