Topological defects in graphene nanostructures

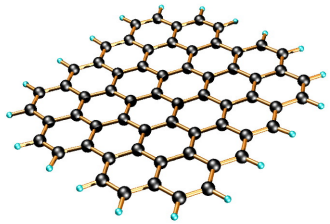
J. Smotlacha

International Conference and Exhibition on Mesoscopic & Condensed Matter Physics

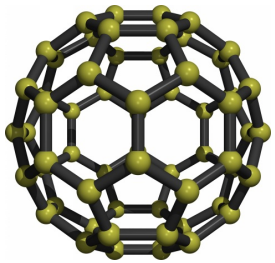
June 22-24, 2015, Boston, USA

Topological defects in graphene nanostructures

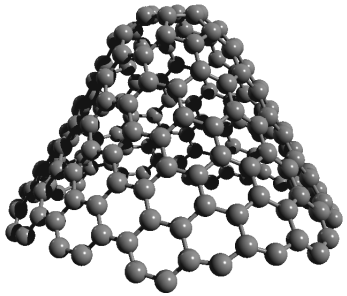
- Carbon Nanostructures:
  - graphene



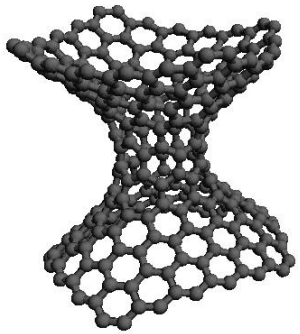
  - fullerene



  - nanocone



  - wormhole

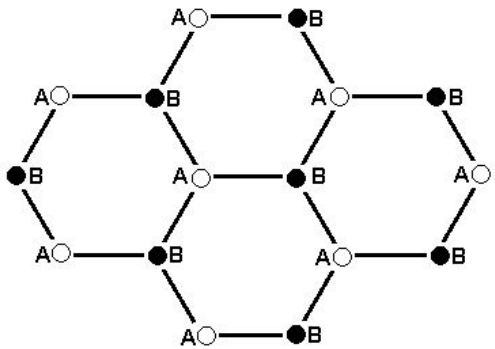


  - nanotubes, nanotoroids, etc.

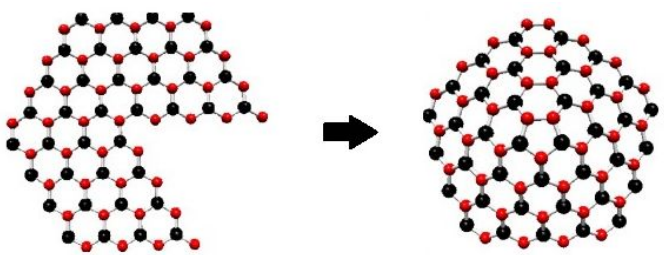
Topological defects in graphene nanostructures

- Basic structure: Hexagonal plane lattice

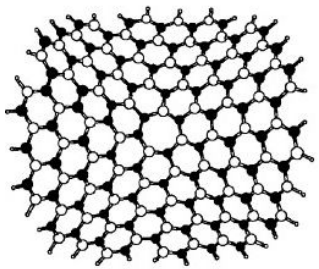
  it is composed of 2 inequivalent sublattices, *A* and *B*



- Topological defects: *n*-sided polygons



$n \leq 5$ (positive curvature)



$n \geq 7$ (negative curvature)

Topological defects in graphene nanostructures

- Electronic properties
  - Important characteristics: Local density of states

    number of states per the unit interval of energy and per the unit area of surface at each energy level that is available to be occupied by electrons
  - Calculation of *LDoS* for low energies:
    - periodical structures: from the low energy electronic spectrum using Schrödinger equation describing the electron motion [1,2]
    - aperiodical structures: from the continuum limit of the gauge field theory using Dirac-like equation describing the motion of massless fermion [3]
    - graphene wormhole: using Dirac-like equation describing the motion of massive fermion [4]

Topological defects in graphene nanostructures

- Periodical structures: plain graphene, nanotubes (continuous spectrum), fullerene, nanoribbons (discrete spectrum)
  - the electron which is bounded on the molecular surface satisfies the Schrödinger equation [1]:

$$H\psi = E\psi, \qquad \psi = C_A\psi_A + C_B\psi_B$$

    where A, B represent the particular sublattices
  - solution: Bloch function $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}u_{\vec{k}}(\vec{r})$, where $u_{\vec{k}}(\vec{r})$ has the lattice periodicity [5]
  - tight-binding approximation:

$$\psi_{A(B)} = \sum_{A(B)} \exp[i\vec{k}\cdot\vec{r}_{A(B)}]X(\vec{r}-\vec{r}_{A(B)}),$$

    where $X(\vec{r})$ is the atomic orbital function (this solution satisfies the Bloch theorem)
  - assumption: $\int X(\vec{r}-\vec{r}_A)X(\vec{r}-\vec{r}_B)\mathrm{d}\vec{r} = 0$

Topological defects in graphene nanostructures

- case of graphene
  - we denote

$$H_{ab} = \int \psi_a^* H \psi_b \mathrm{d}\vec{r}, \qquad S = \int \psi_A^* \psi_A \mathrm{d}\vec{r} = \int \psi_B^* \psi_B \mathrm{d}\vec{r}, \qquad a, b \equiv A, B,$$

  then

$$\begin{pmatrix} H_{AA} & H_{AB} \\ H_{BA} & H_{BB} \end{pmatrix} \begin{pmatrix} C_A \\ C_B \end{pmatrix} = ES \begin{pmatrix} C_A \\ C_B \end{pmatrix}$$

  - the rotational symmetry gives $H_{AA} = H_{BB}$, then, putting $H'_{ab} = H_{ab}/S$, we get from the secular equation

$$E = H'_{AA} \pm |H'_{AB}|$$

  - we consider H'_{AA} to be the Fermi level, then, after substitution the corresponding expansion into H'_{AB}, we get

$$E(\vec{k}) = \pm\gamma_0 \sqrt{1 + 4\cos^2\frac{k_y a}{2} + 4\cos\frac{k_y a}{2}\cos\frac{k_x a\sqrt{3}}{2}},$$

  where

$$\gamma_0 = -\int X^*(\vec{r} - \vec{\rho}) H X(\vec{r}) \mathrm{d}\vec{r},$$

  $\vec{\rho}$ joining the given site A with the nearest site B

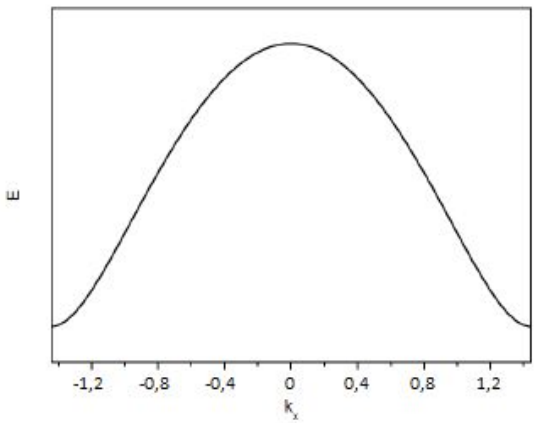
Topological defects in graphene nanostructures

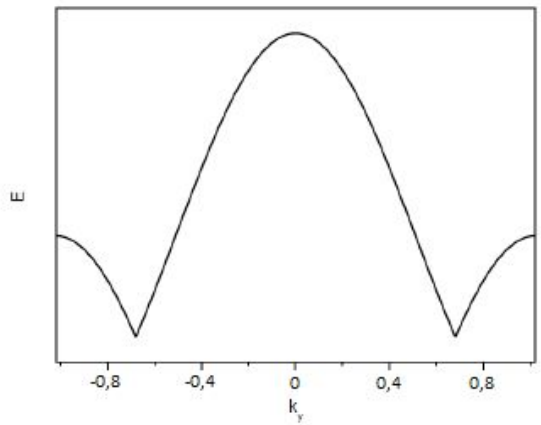
- the *LDoS* we get as

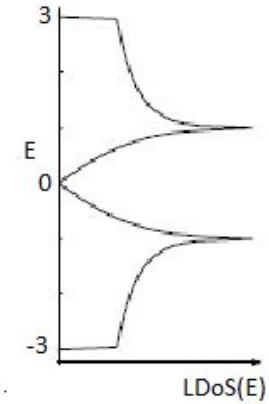
$$LDoS(E,k) = \frac{\delta(E - E(k))}{D(E)},$$

where

$$D(E) = \lim_{\eta \to 0} 2\mathrm{Im} \int_{-\pi}^{\pi} \mathrm{d}k \frac{k}{E - E(k) - i\eta}$$

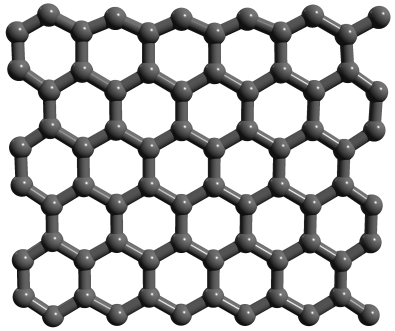




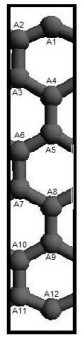


Topological defects in graphene nanostructures

- case of nanoribbon [6]



unit cell:



- matrix elements:

$$H_{ij} = \int \psi^*_{A_i} H \psi_{A_j} \mathrm{d}\vec{r}, \quad S = \int \psi^*_{A_i} \psi_{A_i} \mathrm{d}\vec{r} = \int \psi^*_{A_j} \psi_{A_j} \mathrm{d}\vec{r}, \quad i,j \in \{1,...,n_{max}\},$$

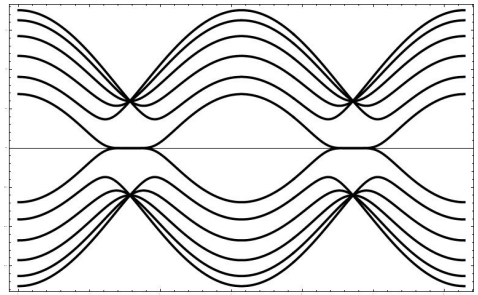
then

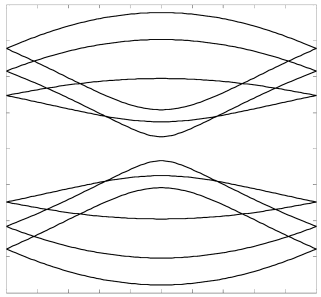
$$\begin{pmatrix} H_{A_1A_1} & H_{A_1A_2} & \dots & \dots & H_{A_1A_{n_{max}}} \\ H_{A_2A_1} & H_{A_2A_2} & \dots & \dots & H_{A_2A_{n_{max}}} \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ H_{A_{n_{max}}A_1} & H_{A_{n_{max}}A_2} & \dots & \dots & H_{A_{n_{max}}A_{n_{max}}} \end{pmatrix} \begin{pmatrix} C_{A_1} \\ C_{A_2} \\ \dots \\ \dots \\ C_{A_{n_{max}}} \end{pmatrix} = ES \begin{pmatrix} C_{A_1} \\ C_{A_2} \\ \dots \\ \dots \\ C_{A_{n_{max}}} \end{pmatrix},$$

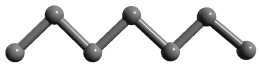
where $H_{A_1A_1} = ... = H_{A_{n_{max}}A_{n_{max}}}$

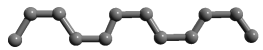
Topological defects in graphene nanostructures

- electronic spectrum:

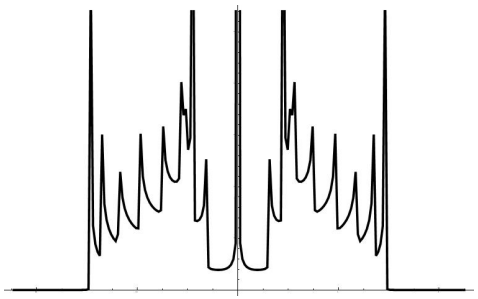


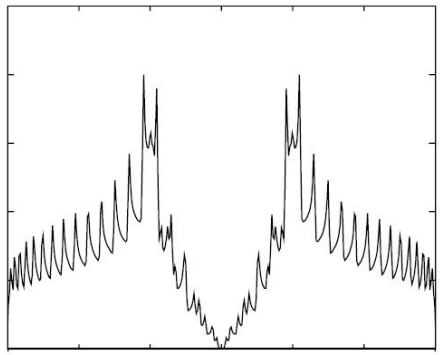


zigzag edge 

armchair edge 

- LDoS:





zigzag

armchair

Topological defects in graphene nanostructures

- Aperiodical structures: close vicinity of the defects, nanocone, wormhole
  - due to the aperiodicity, the eigenfunctions in the Schrödinger equation can't be labelled by the wave-vector $\vec{k}$
  - in the corresponding Hamiltonian, the aperiodicity is present by the potential $U(\vec{r})$, using the $\vec{k} \cdot \vec{p}$ perturbation theory and the continuum gauge field theory, the original Schrödinger equation for the bounded electron is transformed to the Dirac-like equation for the massless fermion [7]

$$i\sigma^{\alpha} e^{\mu}_{\alpha}[\partial_{\mu} + \Omega_{\mu} - ia_{\mu} - ia^{W}_{\mu} - iA_{\mu}]\psi = E\psi, \qquad \psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

  - e^{μ}_{α} - zweibein, ω_{μ} - spin connection,

    $\Omega_{\mu} = \frac{1}{8}\omega^{\alpha\beta}_{\mu}[\sigma_{\alpha}, \sigma_{\beta}]$ - spin connection in the spinor representation

  - a_{μ}, a^{W}_{μ} - ensuring the circular periodicity
  - A_{μ} - magnetic field

- solution:

using the substitution

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \frac{1}{\sqrt[4]{g_{\varphi\varphi}}} \begin{pmatrix} u_j(\xi) e^{i\varphi j} \\ v_j(\xi) e^{i\varphi(j+1)} \end{pmatrix}, \qquad j = 0, \pm 1, ...,$$

so

$$\frac{\partial_\xi u_j}{\sqrt{g_{\xi\xi}}} - \frac{\widetilde{j}}{\sqrt{g_{\varphi\varphi}}} u_j = E v, \qquad -\frac{\partial_\xi v_j}{\sqrt{g_{\xi\xi}}} - \frac{\widetilde{j}}{\sqrt{g_{\varphi\varphi}}} v_j = E u,$$

where

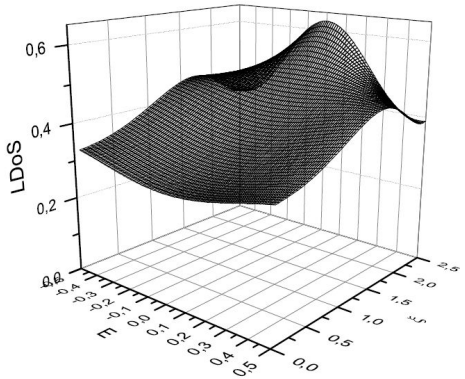
$$\widetilde{j} = j + 1/2 - a_\varphi - a_\varphi^W - A_\varphi,$$

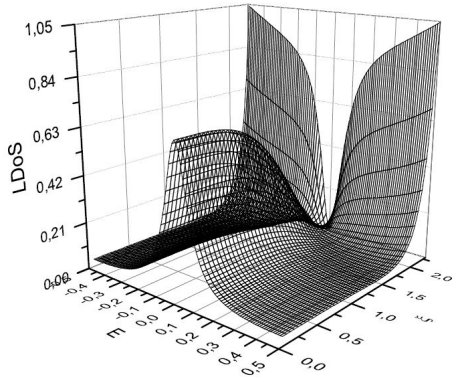
$$g_{\xi\xi}, g_{\varphi\varphi} - \text{the metric coefficients}$$

- $LDoS(E, \xi_0) = u^2(E, \xi_0) + v^2(E, \xi_0)$

Topological defects in graphene nanostructures

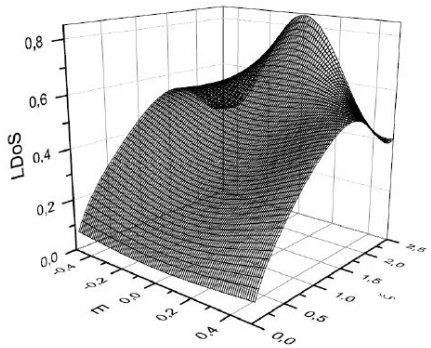
- close vicinity of the defects [7, 10] (hyperboloidal geometry):
  - heptagonal defects (1-fold hyperboloid)

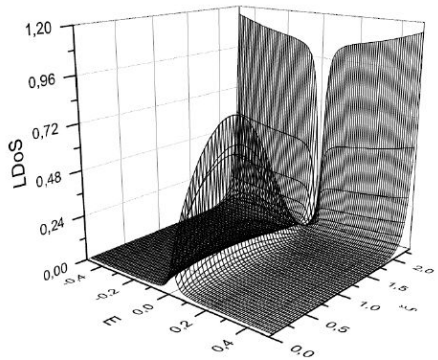




magnetic field: $B = 0$ $B = 0.5\Phi_0$

  - pentagonal defects (2-fold hyperboloid)

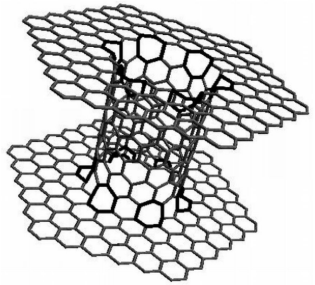




magnetic field: $B = 0$ $B = 0.5\Phi_0$

Topological defects in graphene nanostructures

- case of wormhole [9, 10]:



  - composed of two graphene sheets which are in the places of wormhole bridges connected with the help of very short connecting nanotube
  - described with the help of the polar-like coordinates $r_\pm, \varphi$ satisfying $r_+ r_- = a^2$, where the sign $\pm$ denotes the upper and lower graphene sheet, resp. and a is the wormhole radius
  - metric tensor: $g_{\mu\nu} = \Lambda^2(r_\pm) \begin{pmatrix} 1 & 0 \\ 0 & r_\pm^2 \end{pmatrix}$, where

$$\Lambda(r_\pm) = (a/r_\pm)^2 \, \theta(a - r_\pm) + \theta(r_\pm - a)$$

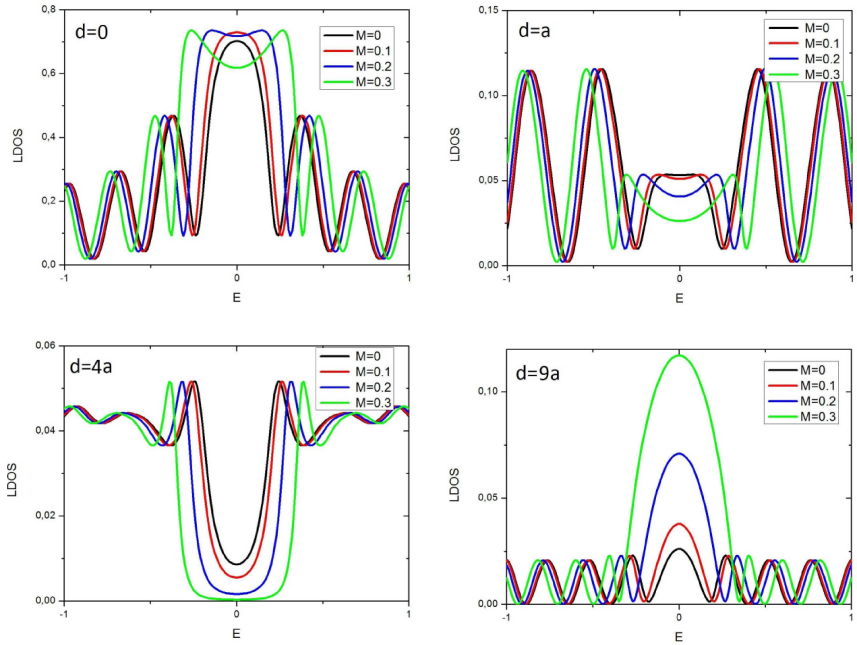
  - due to the relativistic efects, the corresponding Dirac-like equation involves mass terms and using the substitution method, the radial part of the system can be replaced by one differential equation of the form

$$\left(\partial_{\xi\xi} - \frac{1}{2g_{\xi\xi}} \partial_\xi g_{\xi\xi} + \frac{\tilde{j}}{2} \sqrt{\frac{g_{\xi\xi}}{g_{\varphi\varphi}^3}} \partial_\xi g_{\varphi\varphi} - \tilde{j}^2 \frac{g_{\xi\xi}}{g_{\varphi\varphi}} + (E^2 - M^2) g_{\xi\xi} \right) u_j = 0,$$

    where the coordinate ξ stands for $r_\pm$

Topological defects in graphene nanostructures

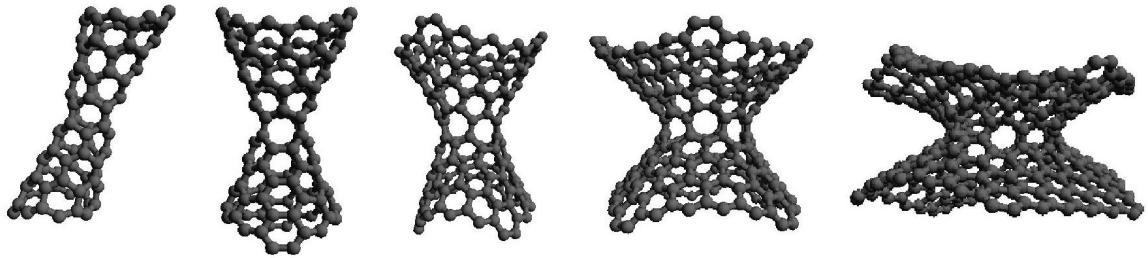
- LDoS:



- spin-orbital interaction:
  comes from the presence of the connecting nanotube, it causes next splitting of the energy levels; because of the presence of the zero modes, as the result, these modes should be detected for the **chiral massive fermions** in the real material - actually, this could serve as a proof of the successful fabrication

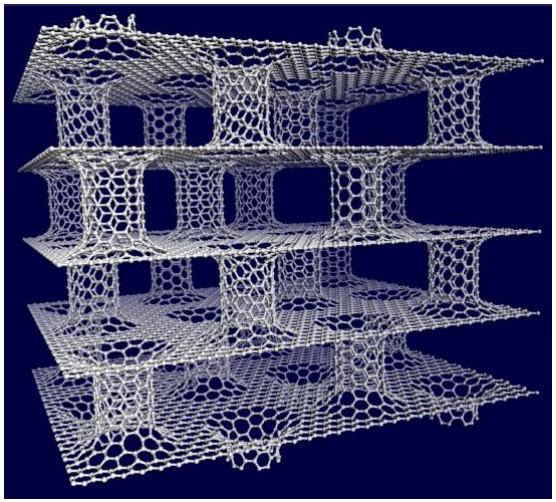
Topological defects in graphene nanostructures

- possible modifications:
  - perturbed wormholes



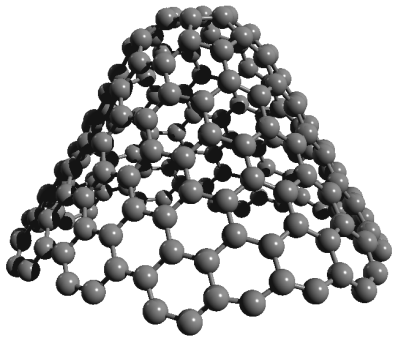
(a) 2 defects, (b) 4 defects, (c) 6 defects, (d) 8 defects, (e) 10 defects

  - pillared graphene



Topological defects in graphene nanostructures

- case of nanocone [11]:



the form of the Hamiltonian is

$\hat{H}_s = \hbar v \left\{ i\sigma^2 \partial_r - \sigma^1 r^{-1} \left[(1-\eta)^{-1} \left(is\partial_\varphi + \frac{3}{2}\eta \right) + \frac{1}{2}\sigma^3 \right] \right\}, s = \pm 1, \eta = \frac{N}{6},$
the solution are the Bessel functions

- involvement of the spin-orbital interaction (SOI) [12]: this interaction is negligible in the plain graphene, but it seems to be significant in the case of graphene nanotubes as well as in the investigated conical structure; we perform the transformations

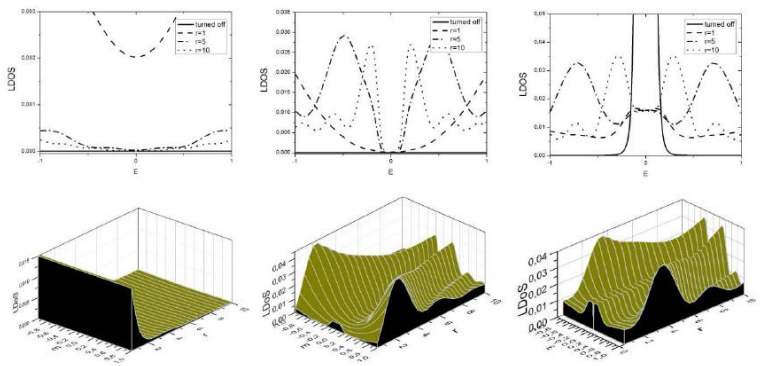
$$\partial_r \to \partial_r \otimes \mathbb{I} - \mathrm{i}\frac{\delta\gamma'}{4\gamma R} \otimes \sigma_x(\vec{r}), \qquad \mathrm{i}\partial_\varphi \to \mathrm{i}\partial_\varphi \otimes \mathbb{I} + s(1-\eta)A_y \otimes \sigma_y$$

Topological defects in graphene nanostructures

- solution: $\psi(r,\varphi) = e^{ij\varphi} \begin{pmatrix} f_{j\uparrow}(r) \\ f_{j\downarrow}(r) \\ g_{j\uparrow}(r) \\ g_{j\downarrow}(r) \end{pmatrix}$, where the radial part must satisfy

$$\begin{pmatrix} 0 & 0 & \partial_r + \frac{F}{r} & -\frac{\mathrm{i}}{r}C \\ 0 & 0 & -\frac{\mathrm{i}}{r}D & \partial_r + \frac{F}{r} \\ -\partial_r + \frac{F-1}{r} & \frac{\mathrm{i}}{r}D & 0 & 0 \\ \frac{\mathrm{i}}{r}C & -\partial_r + \frac{F-1}{r} & 0 & 0 \end{pmatrix} \begin{pmatrix} f_{j\uparrow}(r) \\ f_{j\downarrow}(r) \\ g_{j\uparrow}(r) \\ g_{j\downarrow}(r) \end{pmatrix} = E \begin{pmatrix} f_{j\uparrow}(r) \\ f_{j\downarrow}(r) \\ g_{j\uparrow}(r) \\ g_{j\downarrow}(r) \end{pmatrix}$$

  with $F = \frac{sj}{1-\eta} - \frac{3}{2}\frac{\eta}{1-\eta} + \frac{1}{2}$, $\quad C = \xi_x - \xi_y$, $\quad D = \xi_x + \xi_y$,
  ξ_x, ξ_y - the spin-orbital coefficients
- LDoS:



Topological defects in graphene nanostructures

- finite dimensional case: quantization of the continuous spectrum, the energy shift caused by the SOI can be found with the help of the Green function by the comparison of the LDoS without and with SOI:

$$LDoS(E) = \frac{1}{\pi}\,\mathrm{Im}\,G(E+\mathrm{i}0), \qquad G = G_0 + \int G_0\hat{V}G_0 + \int G_0\hat{V}G_0\hat{V}G_0 + \ldots,$$

where G denotes the case with SOI, $\hat{V}$ stands for the interaction potential of SOI and G_0 which represents the case without SOI has the form

$$G_0(r'',\varphi'',r',\varphi';E) = \frac{1}{2\pi}\sum_{n\in\mathbb{Z}} e^{i(n+s/2)(\varphi''-\varphi')}\mathbb{1}\otimes\begin{pmatrix} a_n^{11}(r'',r') & a_n^{12}(r'',r') \\ a_n^{21}(r'',r') & a_n^{22}(r'',r') \end{pmatrix};$$

$a_n^{kl}(r'',r')$, $k,l=1,2$ are computed in [11]:

$$a_n^{kl}(r'',r') = \int_0^\infty \frac{\mathrm{d}p\,p}{\hbar^2\upsilon^2p^2-E^2}\,a_{n,p}^{kl}(r'',r'),$$

$$a_{n,p}^{11}(r'',r') = 2E\cdot J_{\nu_n}(pr'')J_{\nu_n}(pr'), \quad a_{n,p}^{12}(r'',r') = 2\hbar\upsilon p\cdot J_{\nu_n+1}(pr'')J_{\nu_n}(pr'),$$
$$a_{n,p}^{21}(r'',r') = 2\hbar\upsilon p\cdot J_{\nu_n}(pr'')J_{\nu_n+1}(pr'), \quad a_{n,p}^{22}(r'',r') = 2E\cdot J_{\nu_n+1}(pr'')J_{\nu_n+1}(pr')$$

Topological defects in graphene nanostructures

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Thank you for your attention