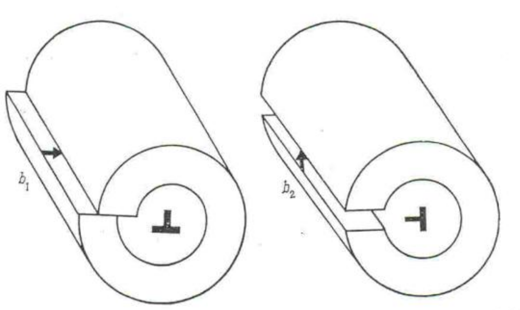
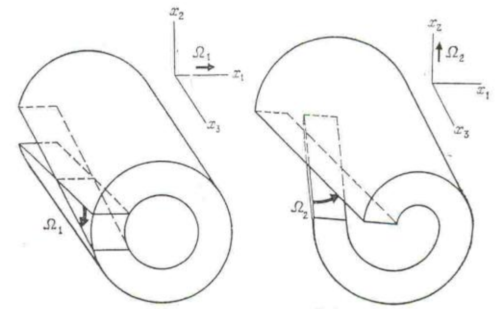
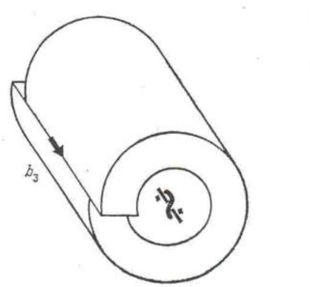
Part 3

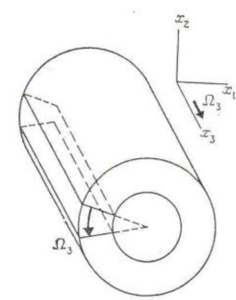
Generic field-theory models

Dislocations and Disclinations









$$\oint\limits_L du_i = \oint\limits_L \frac{\partial u_i}{\partial x_k} dx_k = -b_i.$$

$$\oint\limits_L d\omega_i = \oint\limits_L \frac{\partial \omega_i}{\partial x_k} dx_k = -\Omega_i,$$

$$\vec{u}^P = \vec{u}^+ - \vec{u}^- = \vec{b} + [\vec{\Omega}\vec{R}],$$

$$\vec{\omega} = (1/2) rot \vec{u}$$

Gauge theory of dislocations and disclinations

$$L = L_\chi + L_\phi + L_W$$

$$L_\chi = (\rho_0/2) B_3^i \delta_{ij} B_3^j - [\lambda (E_{AB}\delta^{AB})^2 + 2\mu E_{AB}\delta^{AC}\delta^{BD}E_{CD}]/8$$

$$L_\phi = -(s_1/2)\delta_{ij} D_{ab}^i k^{ac} k^{bd} D_{cd}^j$$

$$L_W = -(s_2/2) F_{ab} g^{ac} g^{bd} F_{cd}$$

Gauge theory

$$E_{AB} = B^i_A \delta_{ij} B^j_B - \delta_{AB}$$

$$B^i_a = \partial_a \chi^i + \epsilon^i_j \chi^j W_a + \phi^i_a$$

$$D^i_{ab} = \partial_a \phi^i_b - \partial_b \phi^i_a + \epsilon^i_j (W_a \phi^j_b - W_b \phi^j_a + F_{ab} \chi^j)$$

$$F_{ab} = \partial_a W_b - \partial_b W_a$$

Gauge theory

$$\partial_3 p_i - \partial_A \sigma_i^A = \epsilon_i^j (W_3 p_j - W_A \sigma_j^A + F_{ab} R_j^{ab})$$

$$\sigma_i^A = (1/2)\delta_B^A \delta_{ij} (\partial_C \chi^j + \epsilon_k^j W_C \chi^k + \phi_C^j)(\lambda \delta^{BC} \delta^{FD} E_{FD} + 2\mu \delta^{RB} \delta^{SC} E_{RS})$$

$$p_i = \rho_0 \delta_{ij} (\partial_3 \chi^j + \epsilon_k^j W_3 \chi^k + \phi_3^j)$$

$$R_i^{ab} = \partial L / \partial D_{ab}^i = -s_1 \delta_{ij} k^{ac} k^{bd} [\partial_c \phi_d^j - \partial_d \phi_c^j + \epsilon_k^j (W_c \phi_d^k - W_d \phi_c^k) + \epsilon_k^j F_{cd} \chi^k]$$

Disclinations only

$$\partial_A \sigma_i^A = \epsilon_i^j W_A \sigma_j^A,$$

$$\partial_A F^{AB} = \frac{1}{2s_2} \epsilon_j^i \sigma_i^B \chi^j.$$

$$\sigma_i^A = \frac{1}{2}\delta_B^A \delta_{ij}(\partial_C \chi^j + \epsilon_k^j W_C \chi^k)(\lambda \delta^{BC} \delta^{FD} E_{FD} + 2\mu \delta^{RB} \delta^{SC} E_{RS})$$

Disclinations only (linear approximation)

$$\partial_A \Sigma_i^A = 0, \qquad \Sigma_j^A = \frac{1}{\mu}\sigma_j^A = \frac{L}{2}\delta_j^A Sp E_{AB} + \delta_j^B E_{AB}.$$
$$\partial_A F^{AB} = 0.$$

$$E_{AB} = \partial_A u^B + \partial_B u^A + \epsilon_C^A W_B x^C + \epsilon_C^B W_A x^C.$$

$$\triangle \vec{u} + (L+1)\nabla div \vec{u} = \vec{j}(\vec{r}).$$

$$j^x(\vec{r}) = L(W_y + x\partial_x W_y) + x\partial_y W_x - (L+2)y\partial_x W_x - y\partial_y W_y - W_y,$$
$$j^y(\vec{r}) = -L(W_x + y\partial_y W_x) - y\partial_x W_y + (L+2)x\partial_y W_y + x\partial_x W_x + W_x.$$

Gauge field

$$W_A = -\nu \epsilon_C^A \frac{x^C}{r^2}.$$

$$W_r(x^B) = 0, \qquad W_\phi(x^B) = W(r) = \frac{\nu}{r},$$

$$\omega = \oint_L \vec{W} d\vec{l} = 2\pi\nu.$$

The problem:

one has to formulate a theoretical model describing electrons on arbitrary curved surfaces with disclinations taken into account.

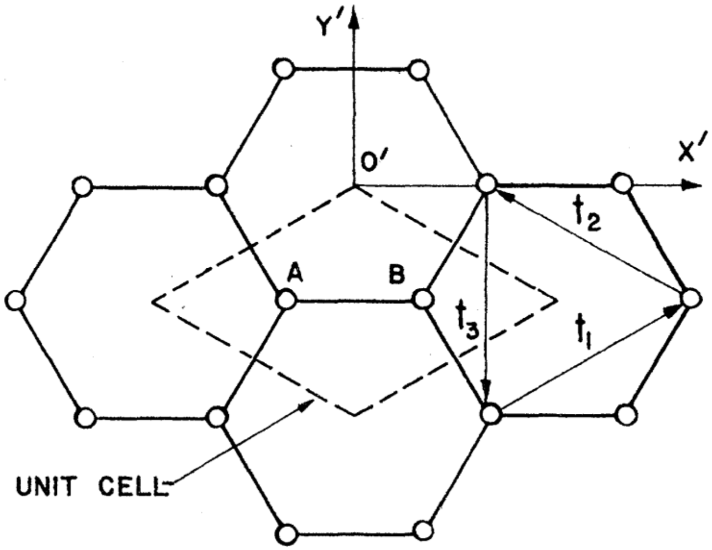
How to start?

As an important basis, one can use the self-consistent effective-mass theory developed for a single hexagonal layer in
P.R. Wallace, Phys.Rev. 71, 622 (1947);
J.C. Slonczewski and P.R. Weiss, Phys. Rev., 109, 272 (1958).

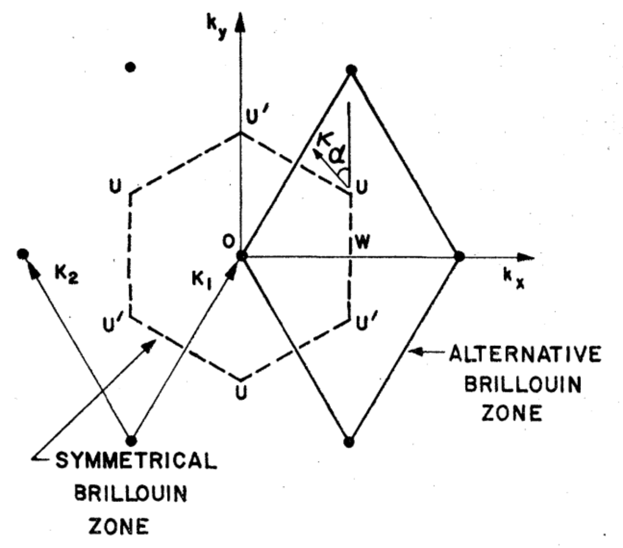
Graphite plane

J.C. Slonczewski and P.R. Weiss, Phys.Rev. 109, 272 (1958)

Real space



Reciprocal space

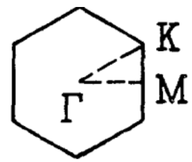


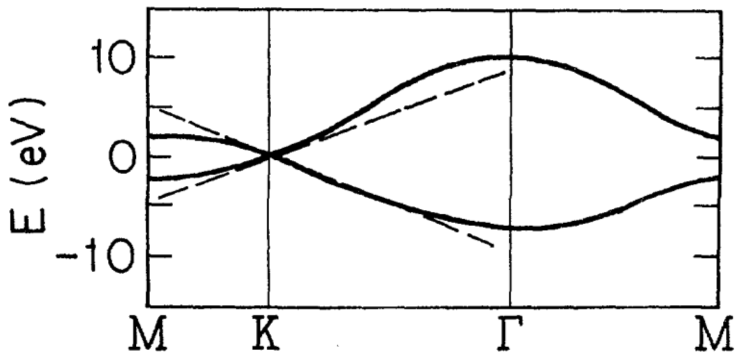
Important:

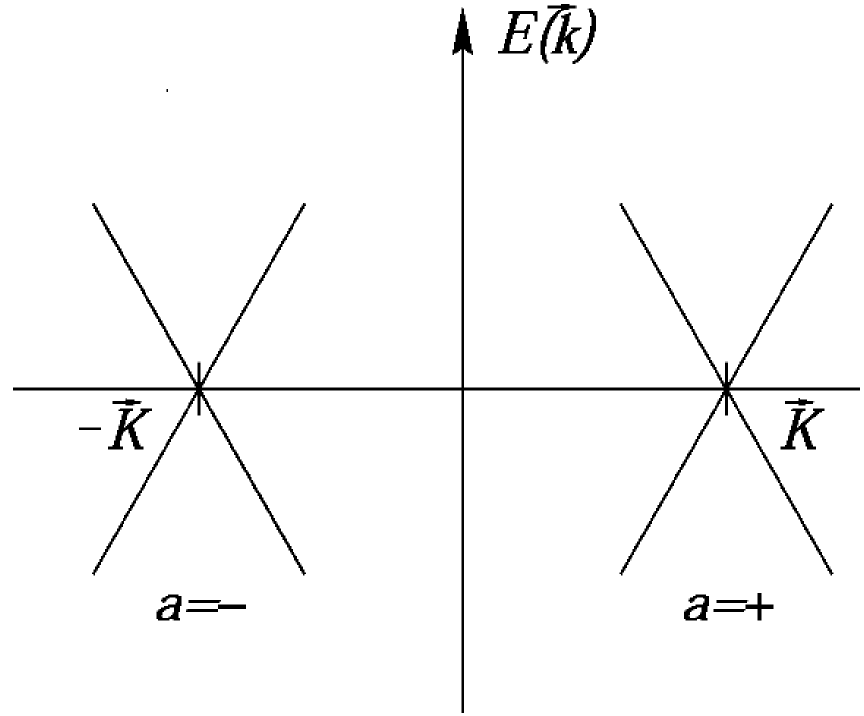
•there are two atoms per unit cell;

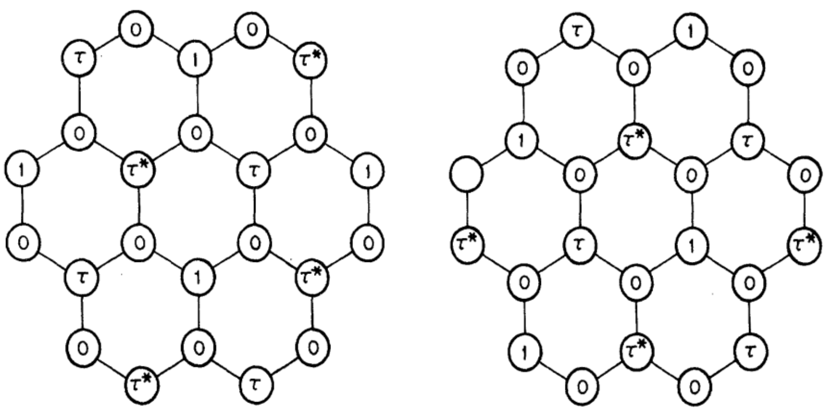
•there are to generate Bloch eigenstates at the Fermi point.

Lattice, spectrum









$\tau = e^{i\frac{2\pi}{3}}$

Energy-band structure of the bands of a two-dimensional graphite layer.

Two degenerate eigenstates which provide the basis set for the **kp** trial wave function.

DOS in 2D

$$DoS(E) = \frac{gV}{4\pi^2} \oint_{\epsilon=E} \frac{dS}{|grad_k \epsilon(\vec{k})|}.$$

g = 4 –degeneracy of electronic states

For linear (Dirac-type) spectrum

$$DoS(E) = \frac{gV|E|}{2\pi},$$

Linear in energy E

Local DOS for arbitrary surface

$$LDoS(E, x) = \Sigma_k |\psi_k(x)|^2 \delta(\epsilon(k) - E)$$

Dirac equation

Step1: the effective-mass approximation, which is equivalent to the kp expansion about the K point in the Brillouin zone

$$\Psi(\vec{k},\vec{r}) = f_1^K(\vec{\kappa})e^{i\vec{\kappa}\vec{r}}\Psi_1^S(\vec{K},\vec{r}) + f_2^K(\vec{\kappa})e^{i\vec{\kappa}\vec{r}}\Psi_2^S(\vec{K},\vec{r}) + ..,$$

Step2: put it in the Schroedinger equation and diagonalize the secular equation for functions f_i. As a result,

$$-i\sigma^\mu\partial_\mu\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

$$\psi = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$

The most important fact is that the electronic spectrum of a single graphite plane linearized around the corners of the hexagonal Brillouin zone coincides with that of the Dirac equation in (2+1) dimensions

In a general form

$$\Psi(\vec{r}) = \psi_A(\vec{K},\vec{r})F_A^K(\vec{r}) + e^{i\chi_1}\psi_B(\vec{K},\vec{r})F_B^K(\vec{r}) +$$

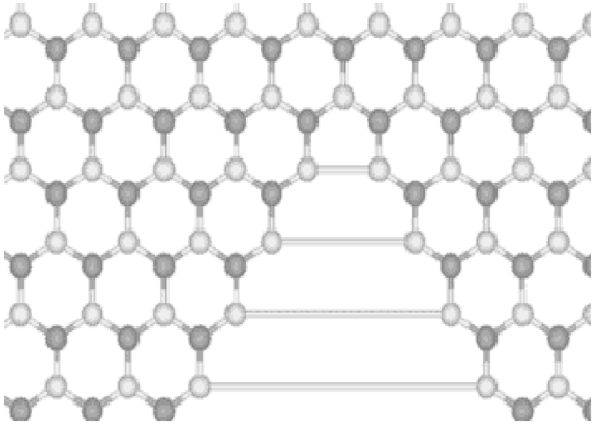
$$+e^{i\chi_2}\psi_A(\vec{K}_-,\vec{r})F_A^{K_-}(\vec{r}) + e^{i\chi_3}\psi_B(\vec{K}_-,\vec{r})F_B^{K_-}(\vec{r}).$$

In the presence of the disclination defect

$$\psi = (F_A^K; F_B^K; F_A^{K_-}; F_B^{K_-}) = \psi(\varphi)$$

$$\psi(\varphi + 2\pi) = -\hat{T}\psi(\varphi)$$

$$\hat{T} = i\tau_2 = e^{i\pi\tau_2/2}$$



$$\oint \vec{a}d\vec{r} = \frac{\pi}{2}\tau_2, \qquad \hat{T} = \exp(i\oint \vec{a}d\vec{r}).$$

This finding stimulated a formulation of some field-theory models for Dirac fermions on hexatic surfaces to describe electronic structure of variously shaped carbon materials:

Fullerenes

J. Gonzalez, F. Guinea and M.A.H. Vozmediano,

Phys. Rev. Lett. **69**, 172 (1992);

Nucl.Phys. B **406**, 771 (1993).

Nanotubes

C.L. Kane and E.J. Mele, Phys. Rev. Lett. **78**, 1932 (1997).

Cones

P.E. Lammert and V.H. Crespi, Phys. Rev. Lett. **85**, 5190 (2000).

Our approach is based on the gauge theory of disclinations on fluctuating elastic surfaces. More particularly, we formulate the Dirac equation on a curved surface with two fluxes due to a pentagonal disclination represented by gauge fields.

Fermions on a curved surface (general)

$$e_\alpha \to e'_\alpha = \Lambda_\alpha^\beta e_\beta,\ \Lambda_\alpha^\beta \in SO(2)$$

Orthonormal frames

$$g_{\mu\nu} = e_\mu^\alpha e_\nu^\beta \delta_{\alpha\beta}$$

zweibain

The gauge field of the local Lorentz group is the spin connection

$$\mathcal{D}_\mu e_\nu^a := \partial_\mu e_\nu^a - \Gamma_{\mu\nu}^\lambda e_\lambda^a + (\omega_\mu)^a{}_b e_\nu^b = 0$$

Covariantly constant

$$(\omega_\mu)^{ab} = e_\nu^a D_\mu e^{b\nu}$$

The model

$$-i\sigma^{\alpha} e_{\alpha}^{\ \mu} (\nabla_{\mu} - i a_{\mu}^{k} - i W_{\mu}) \psi^{k} = E \psi^{k}$$

- Dirac equation on a curved manifold
- Two sorts of spinors
- geometry
- gauge fields

Geometrical characteristics

Covariant derivative

$$\nabla_\mu = \partial_\mu + \Omega_\mu$$

Spin connection term

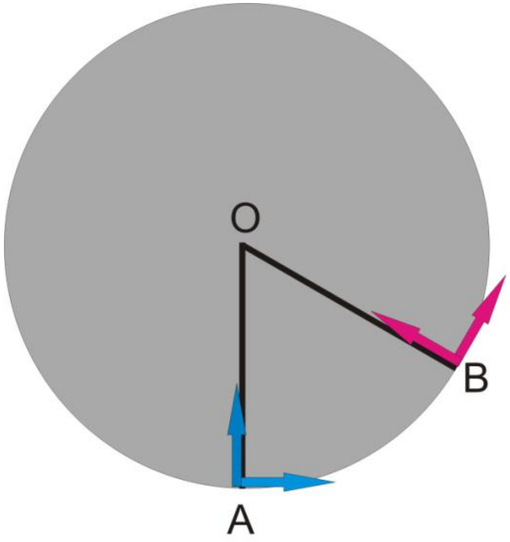
$$\Omega_\mu = (1/8)\omega^{\alpha}{}_{\mu}{}^{\beta}[\sigma_\alpha, \sigma_\beta]$$

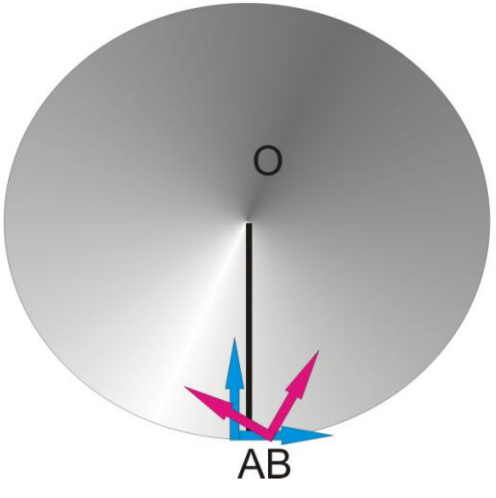
Spin connection coefficients:

$$(\omega_\mu)^{ab} = e^a_\nu(\partial_\mu e^{\nu b} - \Gamma^\nu_{\mu\chi}e^{\chi b}) = -(\omega_\mu)^{ba}$$

Metric connection coefficients

$$\Gamma^\nu_{\mu\lambda} = \frac{g^{\nu\chi}}{2}(\partial_\mu g_{\chi\lambda} + \partial_\lambda g_{\chi\mu} - \partial_\chi g_{\mu\lambda})$$

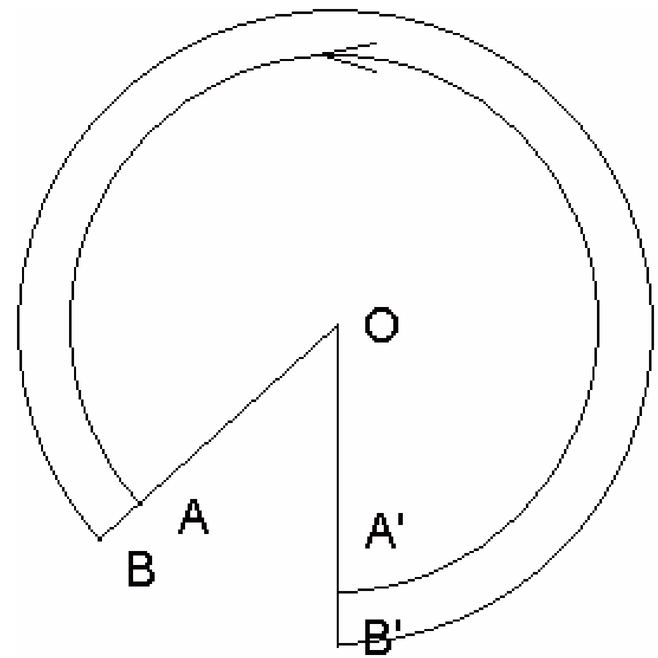




Two gauge fluxes

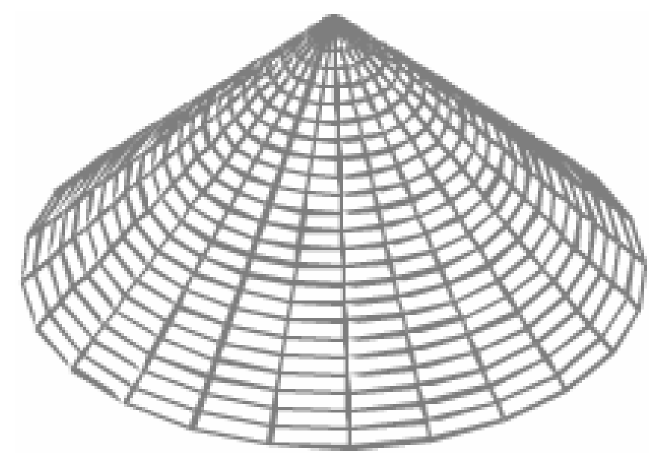
Abelian flux due to a singularity
on elastic surface (adds 1/6)

$$\oint W_\mu dx^\mu = \frac{2\pi}{6}$$



Nonabelian flux due to exchange between
two sublattices for sector angles Nπ/3,
N=2k+1 (adds 1/4 to the total flux)

$$\oint a_\mu dx^\mu = \tau_2 \frac{2\pi}{4}$$

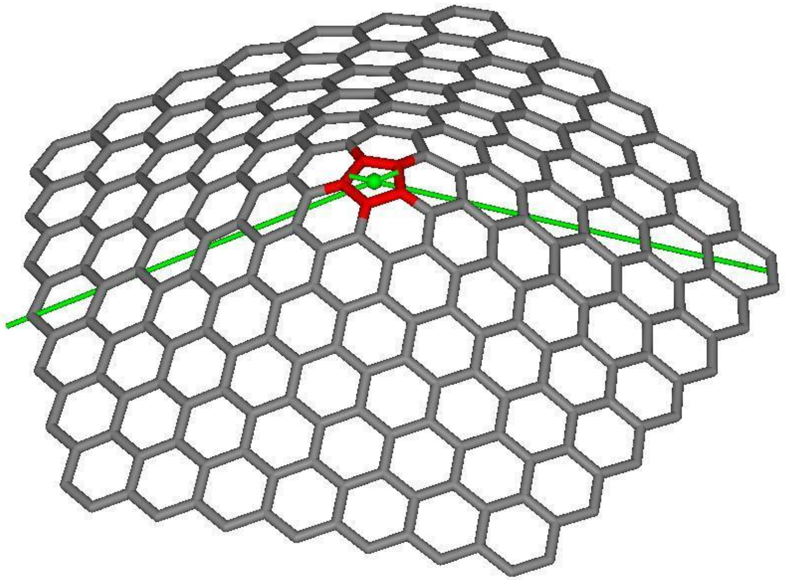


Cone geometry

Due to the symmetry of a graphite sheet only five types of cones can be created from a continuous sheet of graphite. The total disclinations of all these cones are multiplies of 60º, corresponding to the presence of a given number (n) of pentagons at the apices.

Important: carbon nanocones with cone angles of 19º, 39º, 60º, 85º, and 113º have been observed in a carbon sample

A. Krishnan et al., Nature (London), **388**, 451 (1997).



Mathematical exercises

1. choice of appropriate coordinates

$$(r, \varphi) \longrightarrow (ar\cos\varphi, ar\sin\varphi, cr),$$

$$0 < r < 1, \quad 0 \leq \varphi < 2\pi,$$

2. metric tensor

$$g_{rr} = a^2 + c^2, \quad g_{\varphi\varphi} = a^2 r^2, \quad g_{r\varphi} = g_{\varphi r} = 0$$

3. connection

$$\Gamma^r_{\varphi\varphi} = -\frac{r}{\xi}, \quad \Gamma^\varphi_{r\varphi} = \Gamma^\varphi_{\varphi r} = \frac{1}{r}$$

4. zweibeins

$$e^1_r = \sqrt{a^2 + c^2}\cos\varphi, \quad e^1_\varphi = -ar\sin\varphi,$$

$$e^2_r = \sqrt{a^2 + c^2}\sin\varphi, \quad e^2_\varphi = ar\cos\varphi,$$

5. spin connection coefficients

$$\omega^{12}_r = \omega^{21}_r = 0,$$

$$\omega^{12}_\varphi = -\omega^{21}_\varphi = 1 - 1/\sqrt{\xi} =: 2\omega$$

Dirac equations

$$\partial_r \tilde{u} - \frac{\sqrt{\xi}}{r}(j-\nu)\tilde{u} = \tilde{E}\tilde{v},$$

$$-\partial_r \tilde{v} - \frac{\sqrt{\xi}}{r}(j+1-\nu)\tilde{v} = \tilde{E}\tilde{u},$$

$$\psi = \begin{pmatrix} u(r)e^{i\varphi j} \\ v(r)e^{i\varphi(j+1)} \end{pmatrix}$$

$$\tilde{E} = \sqrt{\xi}\, aE.$$

$$\psi = \tilde{\psi} r^{\alpha}, \quad \alpha = \sqrt{\xi}\omega,$$

$$1/\sqrt{\xi} = 1 - \nu$$

General solution

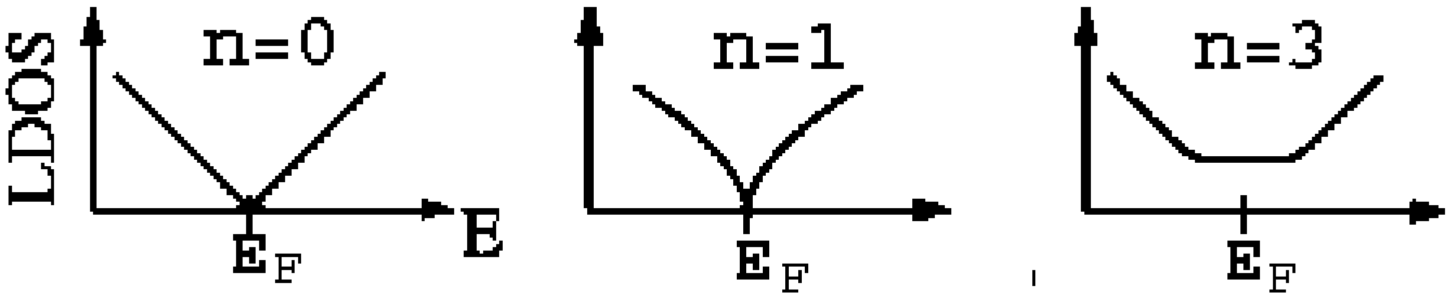
$$\begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} = A r^{-\alpha} \begin{pmatrix} J_{\eta}(\tilde{E} r) \\ \pm J_{\bar{\eta}}(\tilde{E} r) \end{pmatrix}$$

$$\eta = \pm(\sqrt{\xi}(j - \nu + 1/2) - 1/2),$$

$$\bar{\eta} = \pm(\sqrt{\xi}(j - \nu + 1/2) + 1/2).$$

DOS near the apex

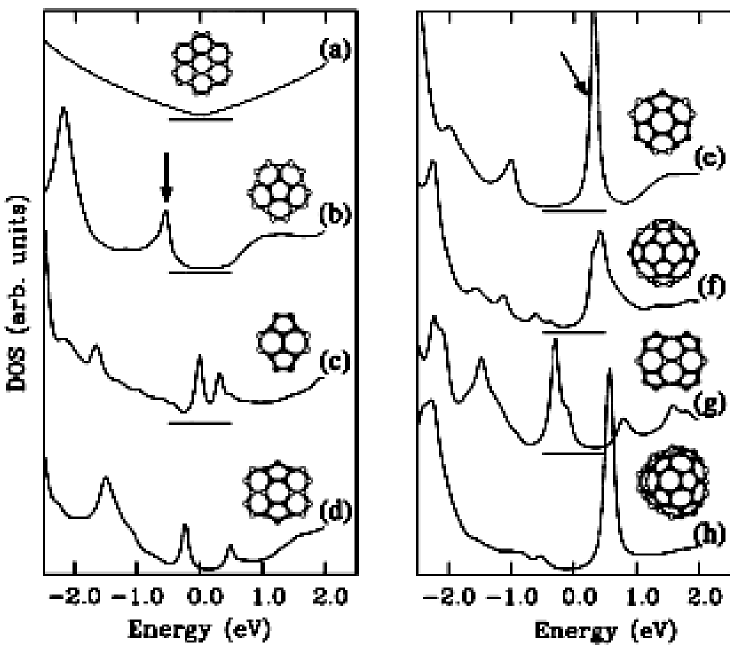
$$D(E,\delta) \propto \begin{cases} E\delta^2, & \nu = 0, \\ E^{4/5}\delta^{9/5}, & \nu = 1/6, \\ E^{1/2}\delta^{3/2}, & \nu = 1/3, \\ \delta, & \nu = 1/2. \end{cases}$$



V. A. Osipov, E. A. Kochetov, and M. Pudlak, JETP 96, 140 (2003)

A presence of sharp resonant states in the region close to the Fermi energy

J.-C. Charlier and G.-M. Rignanese, Phys. Rev.Lett. 86, 5970 (2001)



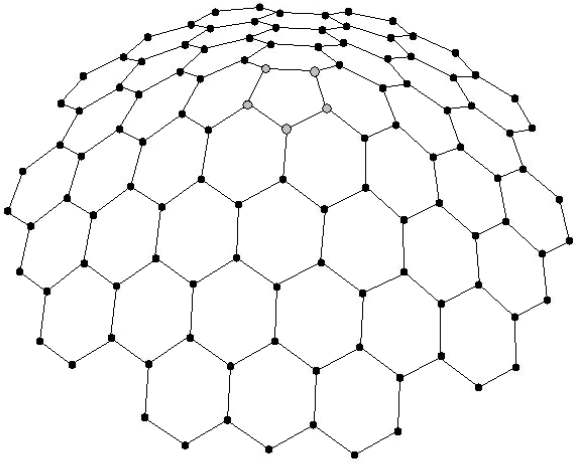
Computed tight-binding LDOS for a single graphene layer (a), and nanocones with one (b), two (c) and (d), three (e), four (f) and (g), and five (h) pentagons, respectively. The Fermi level is at zero energy.

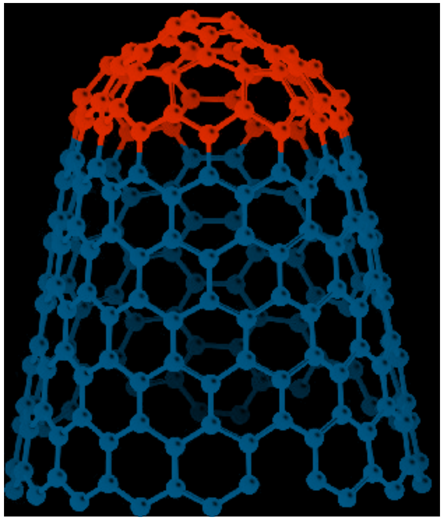
The strength and the position of these states with respect to the Fermi level was found to depend sensitively on the number and the relative positions of the pentagons constituting the conical tip. In particular, a prominent peak which appears just above the Fermi level was found for the nanocone with three symmetrical pentagons (which corresponds to a 60˚ opening angle or, equivalently, to 180˚ disclination).

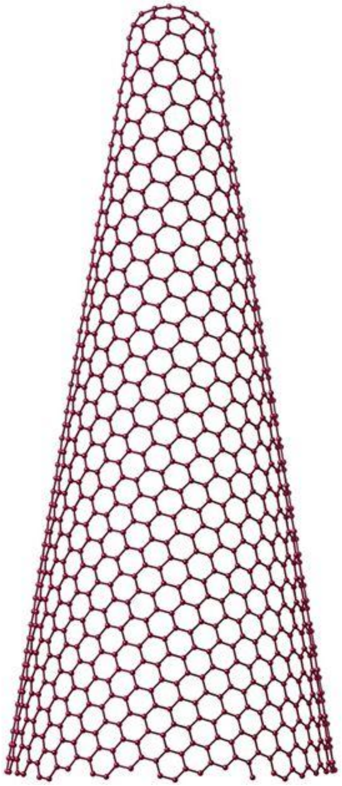
Nanocones: another geometry

Upper half of a two-sheet hyperboloid

$$(\chi, \varphi) \to (a \sinh \chi \cos \varphi, a \sinh \chi \sin \varphi, c \cosh \chi)$$







is suitable for the description of cone-like structures with pentagons situated at a smoothed apex. The most appropriate model for nanohorns with five pentagons at the tip.

$$g_{\chi\chi} = a^2 \cosh \chi^2 + c^2 \sinh \chi^2, \quad g_{\varphi\varphi} = a^2 \sinh \chi^2, \quad g_{\chi\varphi} = 0,$$

$$\Gamma^{\chi}_{\chi\chi} = \frac{(a^2 + c^2) \sinh 2\chi}{2 g_{\chi\chi}}, \quad \Gamma^{\chi}_{\varphi\varphi} = -\frac{a^2 \sinh 2\chi}{2 g_{\chi\chi}}, \quad \Gamma^{\varphi}_{\chi\varphi} = \Gamma^{\varphi}_{\varphi\chi} = \coth \chi,$$

$$e^1{}_{\chi} = \sqrt{g_{\chi\chi}} \cos \varphi, \quad e^2{}_{\chi} = \sqrt{g_{\chi\chi}} \sin \varphi,$$

$$e^1{}_{\varphi} = -a \sinh \chi \sin \varphi, \quad e^2{}_{\varphi} = a \sinh \chi \cos \varphi,$$

$$\omega^{12}_{\chi} = \omega^{21}_{\chi} = 0, \quad \omega^{12}_{\varphi} = -\omega^{21}_{\varphi} = \frac{1}{2} \left[1 - \frac{a \cosh \chi}{\sqrt{g_{\chi\chi}}} \right] = \omega,$$

$$W_{\chi} = a_{\chi} = 0, \, W_{\varphi} = N/6 = \nu \ , \ a_{\varphi} = \pm(N/4 + 2M/3)$$

Dirac operator

$$\hat{\mathcal{D}} = \begin{bmatrix} 0 & e^{-i\varphi}\left(-\frac{\partial_\chi}{\sqrt{g_{\chi\chi}}} + \frac{1}{a\sinh\chi}(i\partial_\varphi + \nu + a_\varphi + \omega)\right) \\ e^{i\varphi}\left(\frac{\partial_\chi}{\sqrt{g_{\chi\chi}}} + \frac{1}{a\sinh\chi}(i\partial_\varphi + \nu + a_\varphi - \omega)\right) & 0 \end{bmatrix}$$

$$\psi = \frac{1}{\sqrt{2\pi}}\begin{pmatrix} ue^{ij\varphi} \\ ve^{i(j+1)\varphi} \end{pmatrix}, \; j = 0, \pm 1, \ldots$$

$$\begin{pmatrix} \tilde{u} \\ \tilde{v} \end{pmatrix} = \begin{pmatrix} u \\ v \end{pmatrix} \sqrt{\sinh\chi}$$

Equations, zero modes

$$\partial_\chi \tilde{u} - \sqrt{\coth^2\chi + b^2}\,\Phi\tilde{u} = \tilde{E}\tilde{v},$$

$$-\partial_\chi \tilde{v} - \sqrt{\coth^2\chi + b^2}\,\Phi\tilde{v} = \tilde{E}\tilde{u},$$

$$\tilde{E} = \sqrt{g_{\chi\chi}}\,E,\; b = c/a,\;\; \Phi = j - N/6 + 1/2 \mp N/4 - M/3.$$

$$\tilde{u}_0(\chi) = A\left[(k\cosh\chi + \Delta)^{2k}\,\frac{\Delta - \cosh\chi}{\Delta + \cosh\chi}\right]^{\frac{\Phi}{2}}$$

$$\tilde{v}_0(\chi) = A\left[(k\cosh\chi + \Delta)^{2k}\,\frac{\Delta - \cosh\chi}{\Delta + \cosh\chi}\right]^{-\frac{\Phi}{2}}$$

$$k = \sqrt{1 + b^2};$$

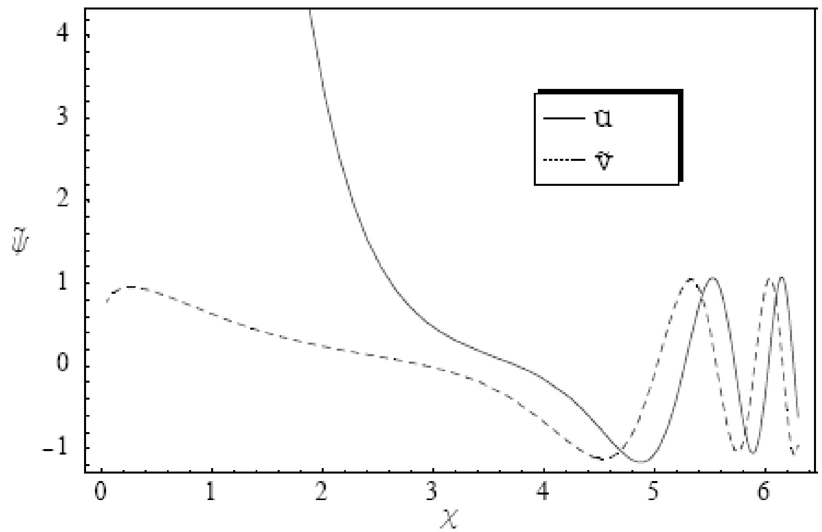
$$\Delta = \Delta(\chi) = \sqrt{1 + k^2\sinh^2\chi}$$

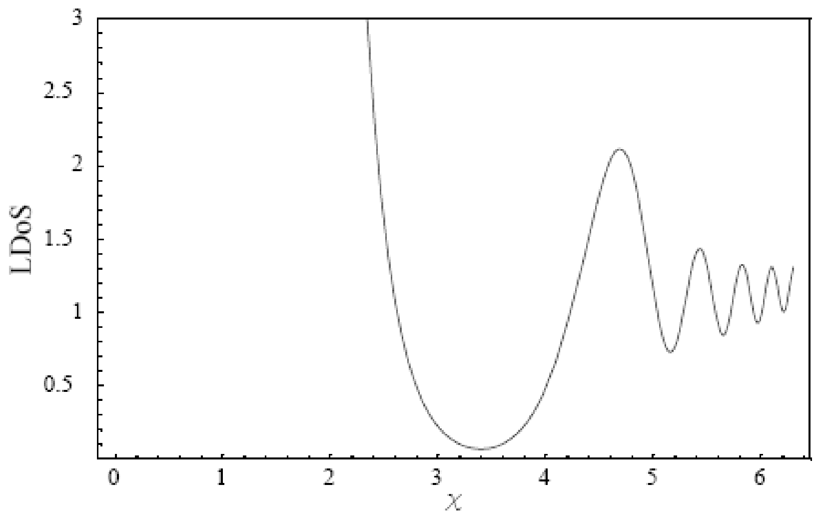
$$k = 1/(1 - N/6)$$

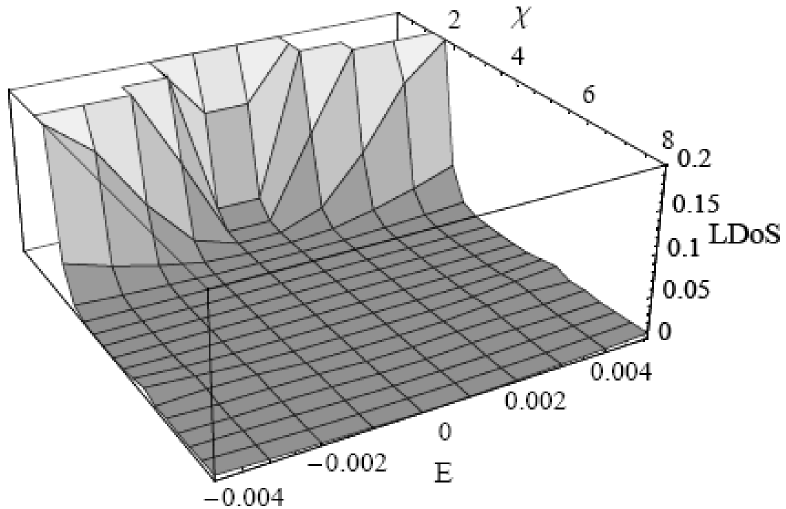
Only $\tilde{v}_0$ **is normalized and only for** $j = 2$ **and** $4 < N < 6.$

Results

D.V. Kolesnikov and V.A. Osipov, JETP Letters, 79, 532 (2004)



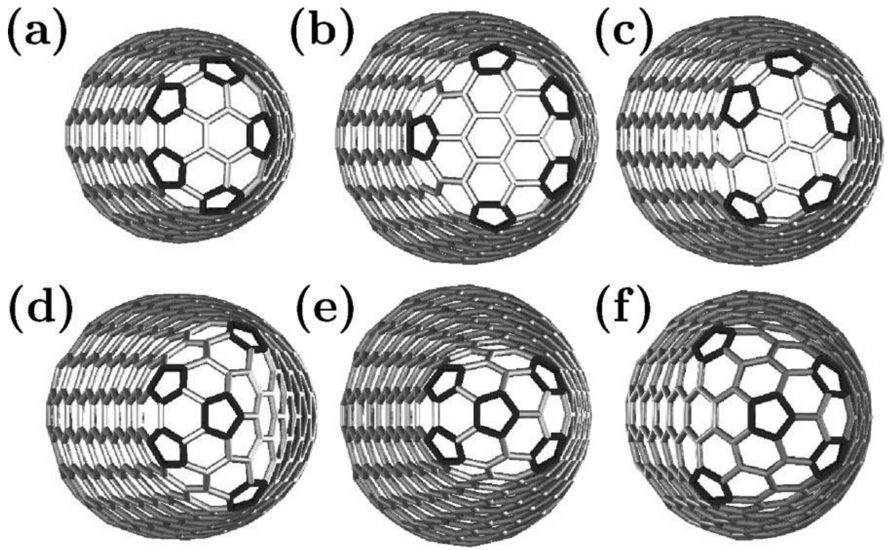


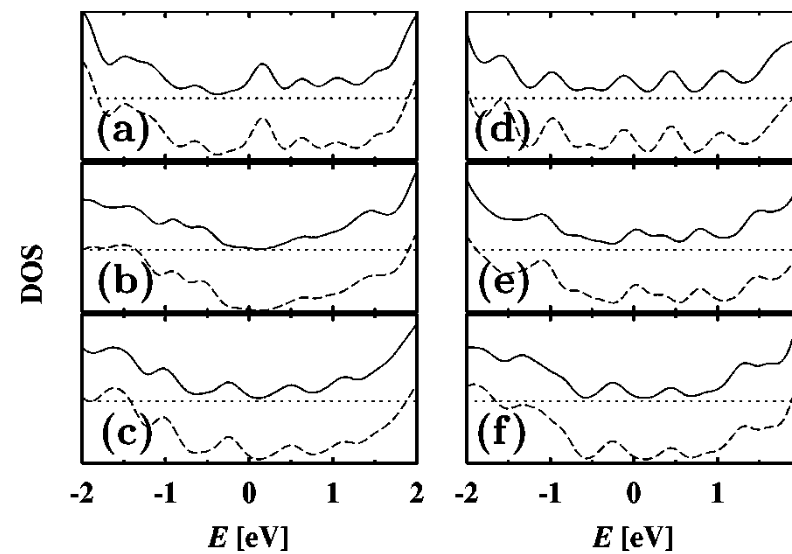


- there exists a normalized zero-mode state
- there is a substantial growth of the normalizable component of the eigenfunction near the defect
- LDoS grows near the Fermi energy and has a distinct non-zero minimum at the Fermi energy

Nanohorns: LCAO calculations

Source: S. Berber et al., Phys.Rev.B 62, R2291 (2000)





Carbon nanohorn structures with a total disclination angle of 5(π/3), containing five isolated pentagons at the terminating cap. Structures (a)–(c) contain all pentagons at the conical “shoulder,” whereas structures (d)–(f) contain a pentagon at the apex.

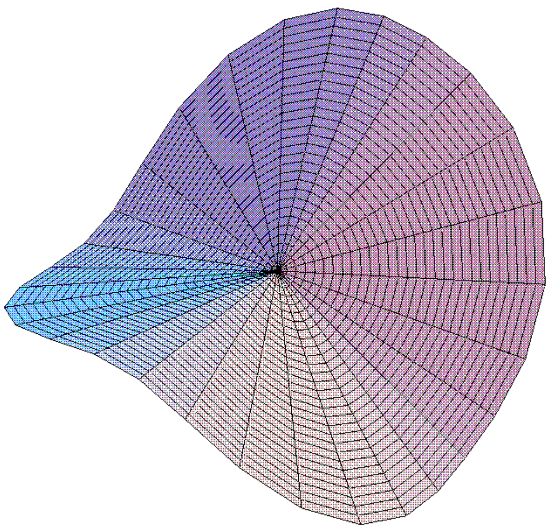
Electronic properties of graphene with negative curvature

D.V.Kolesnikov and V.A.Osipov

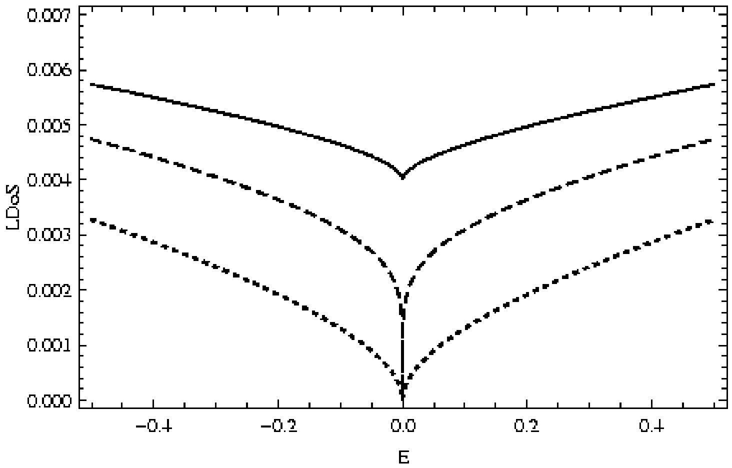
JETP Letters 87, p. 419 (2008)

A gauge field-theory model:

$$-i\sigma^a e_a^\mu(\nabla_\mu - ia_\mu^k - iW_\mu)\psi^k = E\psi^k$$



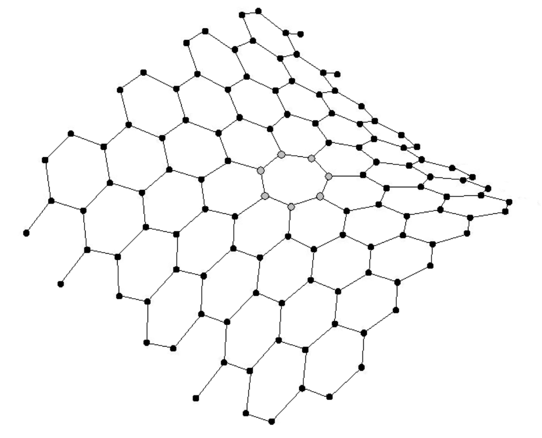
The graphene sixfold lattice with a single sevenfold (negative curvature) at the center



For the specific morphology of two sewenfolds (solid curve), local metallization was found.

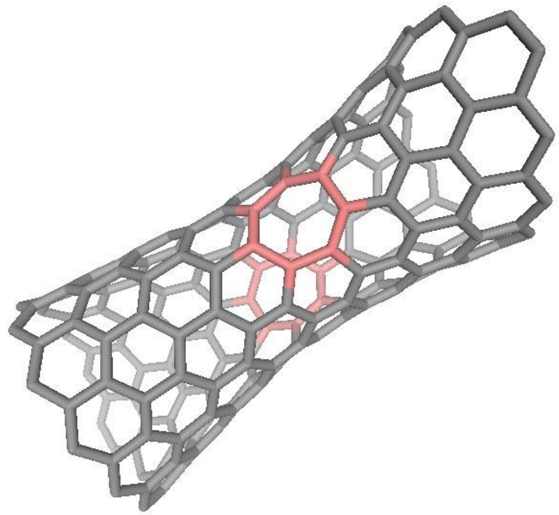
Heptagons: one-sheet hyperboloid

This geometry is suitable for the description of a nanotube containing two or more circularly distributed negative disclinations (heptagons)



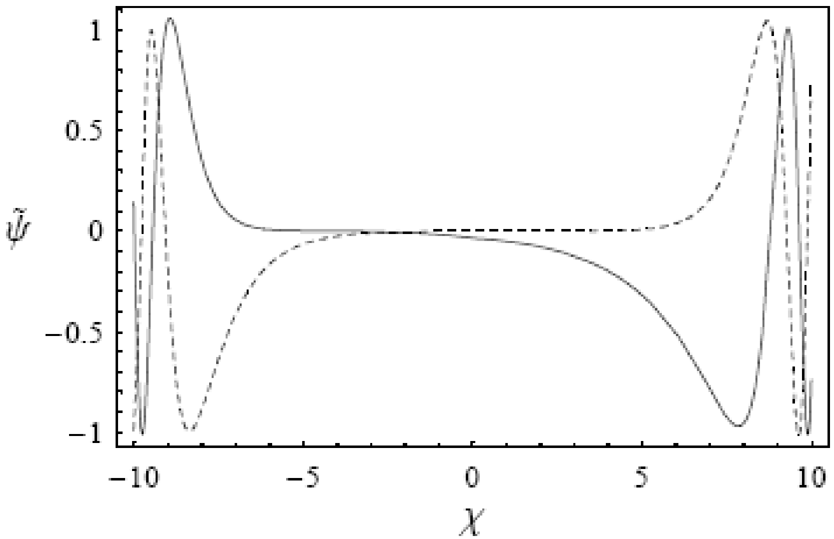
$$(\chi, \varphi) \to (a \sinh\chi \cos\varphi, a \sinh\chi \sin\varphi, c \cosh\chi)$$

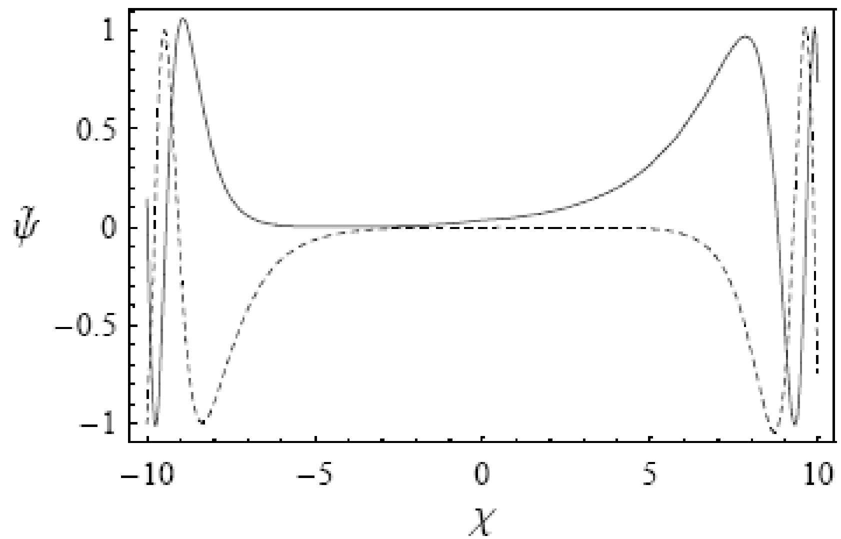
$b=c/a$, $\Phi=\Phi(j,n)$

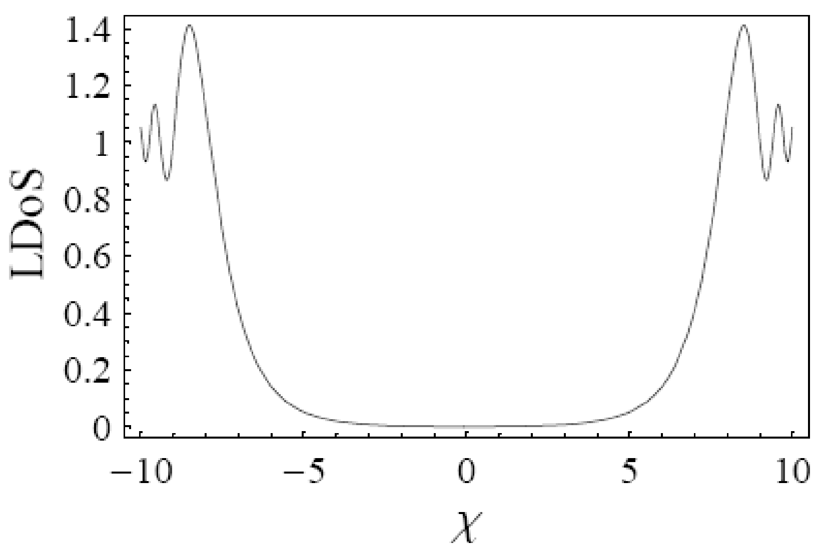


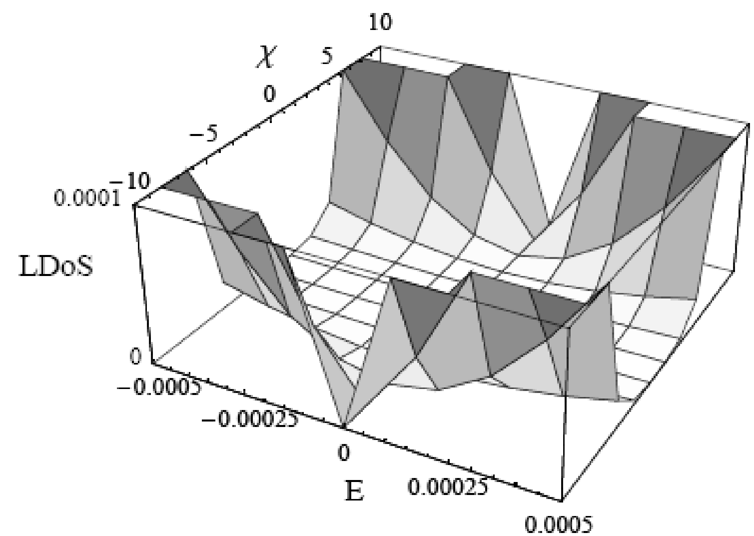
$$\partial_\chi \tilde{u} - \sqrt{\tanh^2\chi + b^2}\,\Phi\tilde{u} = \tilde{E}\tilde{v},$$
$$-\partial_\chi \tilde{v} - \sqrt{\tanh^2\chi + b^2}\,\Phi\tilde{v} = \tilde{E}\tilde{u}$$

Results (two heptagons)

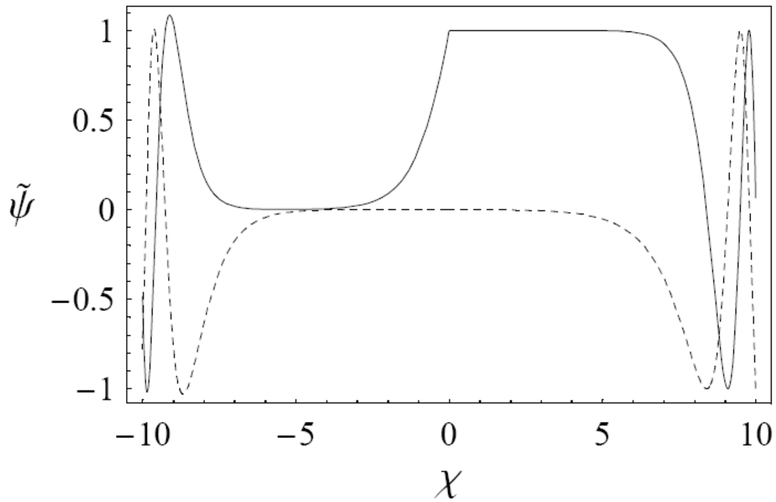


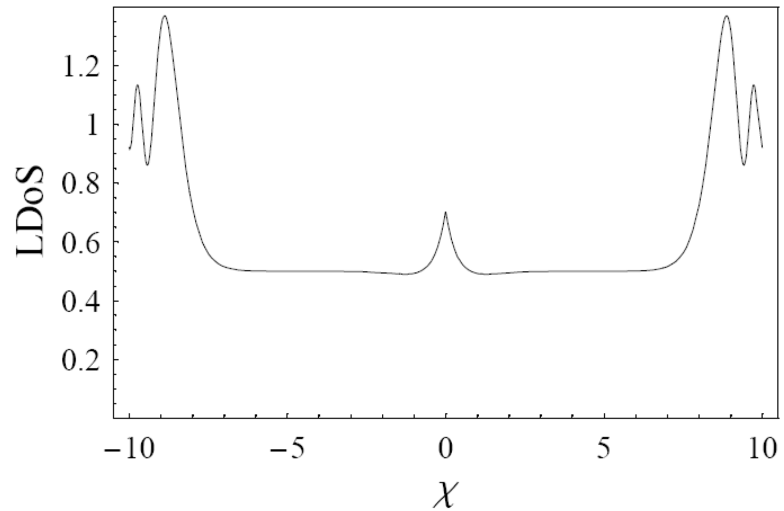


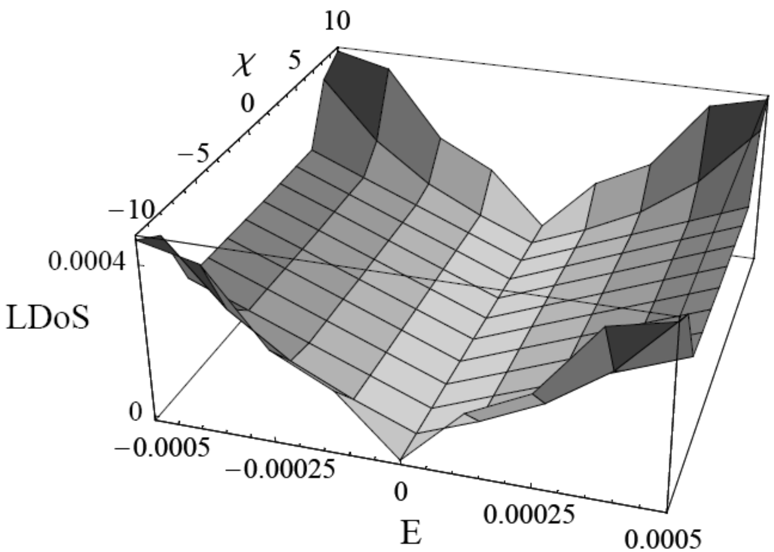




Results (2π negative disclination)



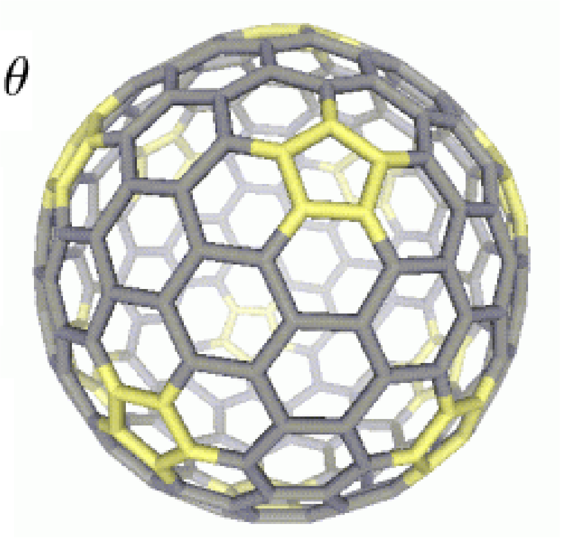




- LDoS decreases markedly near disclinations.
- For six heptagons (2π disclination) the decrease of LDoS has a minimal value. LDoS becomes proportional to energy almost everywhere.
- LDoS at the Fermi energy is found to be zero

Spherical fullerenes

$$g_{\theta\theta} = 1, \quad g_{\varphi\varphi} = \sin^2\theta, \quad e^1{}_\theta = 1, \quad e^2{}_\varphi = \sin\theta$$



C$_{240}$

$$\hat{\mathcal{D}} = -i\sigma_x\left(\partial_\theta + \frac{\cot\theta}{2}\right) - i\frac{\sigma_y}{\sin\theta}(\partial_\varphi - iA\cos\theta)$$

$$\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \sum_j \frac{e^{ij\varphi}}{\sqrt{2\pi}} \begin{pmatrix} u_j(\theta) \\ v_j(\theta) \end{pmatrix}, \qquad j = 0, \pm 1, \pm 2, \ldots$$

$$a_\theta = 0, a_\varphi = \pm\frac{3}{2}\cos\theta, \quad W_\theta = 0, W_\varphi = -\cos\theta.$$

$$A = \pm(a_\varphi^k + W_\varphi)/\cos\theta = \pm 1/2, \pm 5/2$$

Dirac equations

$$-i\left(\partial_\theta + \left[\frac{1}{2} - A\right]\cot\theta + \frac{j}{\sin\theta}\right)v_j(\theta) = Eu_j(\theta),$$
$$-i\left(\partial_\theta + \left[\frac{1}{2} + A\right]\cot\theta - \frac{j}{\sin\theta}\right)u_j(\theta) = Ev_j(\theta).$$

$$\hat{\mathcal{D}}^2 = -\left[\sigma_x\left(\partial_\theta + \frac{\cot\theta}{2}\right) + i\frac{\sigma_y}{\sin\theta}\left(j - A\cos\theta\right)\right]^2 =$$
$$= -\frac{1}{\sin\theta}\partial_\theta\sin\theta\partial_\theta + \frac{1}{4} + \frac{\frac{1}{4} + j^2 + \sigma_z A}{\sin^2\theta} -$$
$$-\frac{\cot\theta}{\sin\theta}\left(\sigma_z j + 2jA\right) + A^2\cot^2\theta,$$

$$\hat{\mathcal{D}}^2\psi = E^2\psi$$

Substitution $$x = \cos\theta$$

$$\left[\partial_x (1-x^2)\partial_x - \frac{(j-Ax)^2 - j\sigma_z x + \frac{1}{4} + \sigma_z A}{1-x^2}\right] \times$$
$$\times \begin{pmatrix} u_j(x) \\ v_j(x) \end{pmatrix} = -(E^2 - \frac{1}{4}) \begin{pmatrix} u_j(x) \\ v_j(x) \end{pmatrix}$$

Substitution

$$\begin{pmatrix} u_j \\ v_j \end{pmatrix} = \begin{pmatrix} (1-x)^{\alpha}(1+x)^{\beta}\tilde{u}_j(x) \\ (1-x)^{\gamma}(1+x)^{\delta}\tilde{v}_j(x) \end{pmatrix}$$

$$\alpha = \frac{1}{2}\left|j - A - \frac{1}{2}\right|, \quad \gamma = \frac{1}{2}\left|j - A + \frac{1}{2}\right|$$
$$\beta = \frac{1}{2}\left|j + A + \frac{1}{2}\right|, \quad \delta = \frac{1}{2}\left|j + A - \frac{1}{2}\right|$$

$$(1-x^2)\partial_x^2\tilde{u}_j + (2(\beta-\alpha) -$$
$$-2(\alpha+\beta+1)x)\partial_x\tilde{u}_j + [-2\alpha\beta - \alpha - \beta -$$
$$-\frac{1}{2}(j^2 - A^2 + \frac{1}{4} - A) + E^2 - \frac{1}{4}]\tilde{u}_j = 0.$$

Jacobi equation

$$(1-x^2)y'' + (\mathcal{B} - \mathcal{A} - (\mathcal{A}+\mathcal{B}+2)x)y' + \lambda_n y = 0,$$
$$\lambda_n = n(n+\mathcal{A}+\mathcal{B}+1),$$

$\mathcal{A} = 2\alpha,\ \mathcal{B} = 2\beta,$ n=0,1,2…

Quantization condition

$$\lambda_n = n(n+2(\alpha+\beta)+1) = -2\alpha\beta - \alpha - \beta -$$
$$-\frac{1}{2}(j^2 - A^2 + \frac{1}{4} - A) + E^2 - \frac{1}{4}.$$

Exact solution

$$u_j = C_u(1-x)^{\alpha}(1+x)^{\beta}P_n^{2\alpha,2\beta},$$
$$v_j = C_v(1-x)^{\gamma}(1+x)^{\delta}P_n^{2\gamma,2\delta},$$

Spectrum

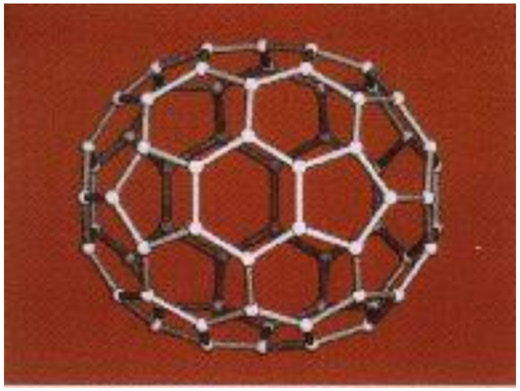
$$E_n^2 = (n+|j|+1/2)^2 - A^2,$$

The unit of energy is $\hbar V_F/R$

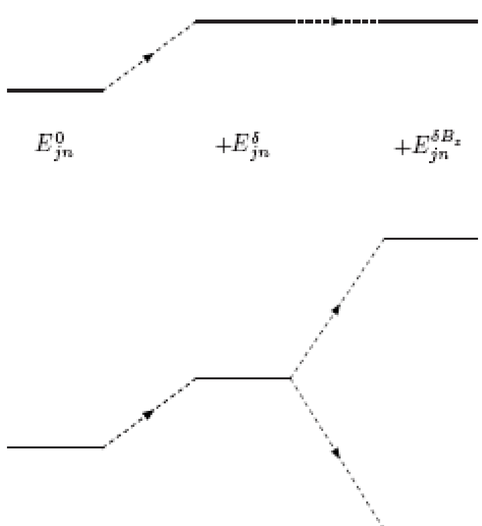
Zero mode

$$u_0 = 0, \qquad v_0 = C_v(1-x)^{\gamma}(1+x)^{\delta},$$

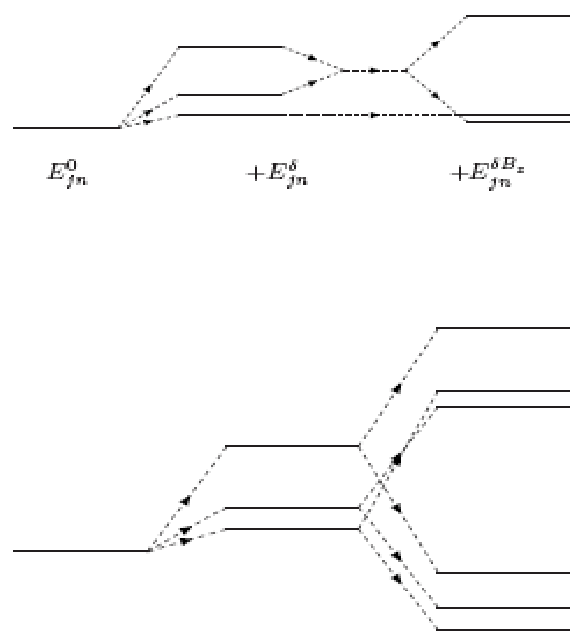
Low-energy electronic states of spheroidal fullerenes in a weak uniform magnetic field



M.Pudlak, R.Pincak and V.A.Osipov,
Phys. Rev. A 75, 025201 (2007)
Phys. Rev. A 75, 065201 (2007)



Zeeman splitting



The first electronic level

The second electronic level

magnetic field is pointed in the *x* (top) and *z* (bottom) directions

Open nanotube (n,m)

$$-i\sigma_1\partial_z\psi(z) + \sigma_2 m\psi(z) = E\psi$$

$$m = -(j - a_\varphi)/R_t$$

$$a_\varphi = \pm M/3$$

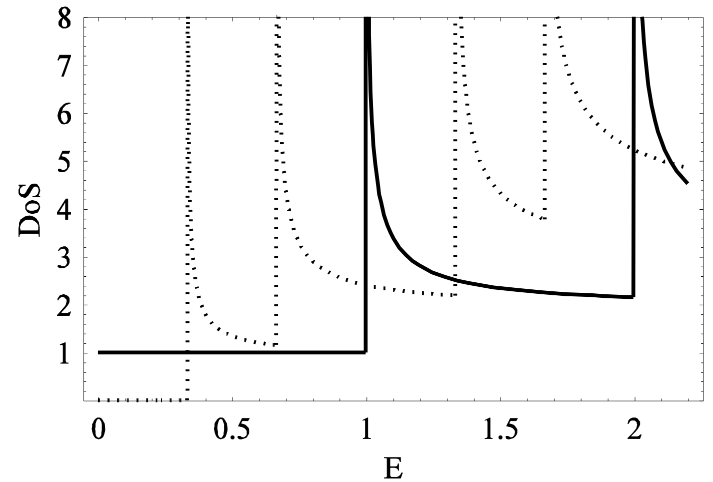
$$M = (n-m)\, mod\, 3$$

The unit of energy is $\hbar V_F/R_t$.

For $(n-m)\, mod\, 3 = 0$ nanotube is metallic

Spectrum $E = \pm\sqrt{k^2 + m^2}$.

Van Hove singularites



$$DoS(E) \sim \left(\frac{\partial E(k)}{\partial k}\right)^{-1}\Big|_{E^2=k^2+m^2} = \frac{E}{\sqrt{E^2 - m^2}}.$$

Closed nanotube

Manifold

$$\vec{R}(\rho(z)\cos\varphi, \rho(z)\sin\varphi, z),\ \ \rho(z) = R_t\sqrt{1-\exp(-2\Lambda)},$$

$$\Lambda = \frac{z+R_f}{R_f},\ \alpha = R_t/R_f,\ z \geq -R_f,\ 0 \leq \varphi < 2\pi,$$

Metric tensor

$$g_{zz} = \alpha^2\frac{e^{-4\Lambda}}{1-e^{-2\Lambda}} + 1, \quad g_{\varphi\varphi} = \rho^2(z), \quad g_{z\varphi} = 0.$$

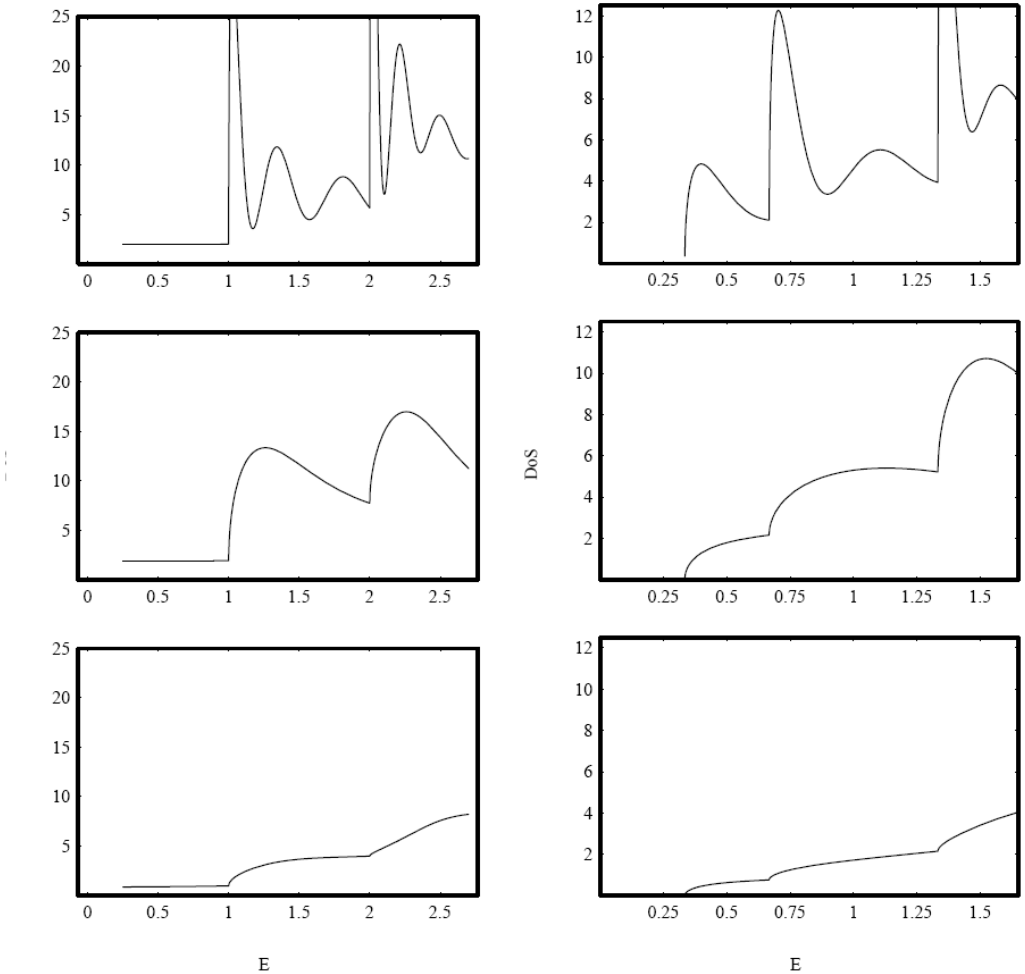
Dirac equation

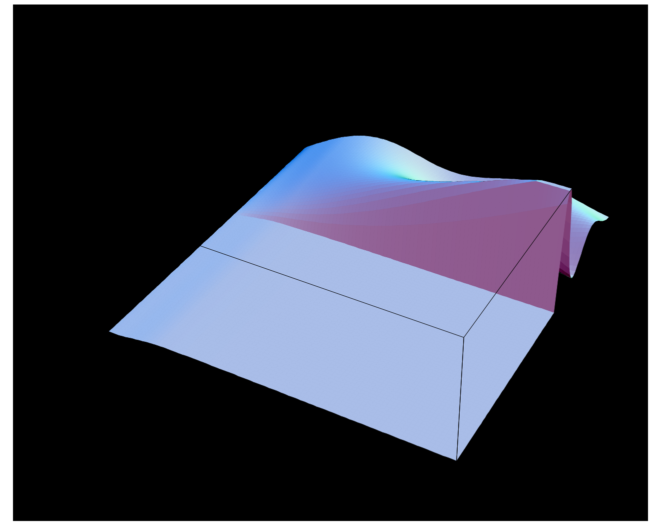
$$-i\left(\frac{\partial_z}{\sqrt{g_{zz}}} + \frac{1}{\rho(z)}\left(j - \frac{\alpha R_t e^{-2\Lambda}}{\rho(z)\sqrt{g_{zz}}} - W_\varphi - a_\varphi\right)\right)v = Eu,$$
$$-i\left(\frac{\partial_z}{\sqrt{g_{zz}}} - \frac{1}{\rho(z)}\left(j + \frac{\alpha R_t e^{-2\Lambda}}{\rho(z)\sqrt{g_{zz}}} - W_\varphi - a_\varphi\right)\right)u = Ev.$$

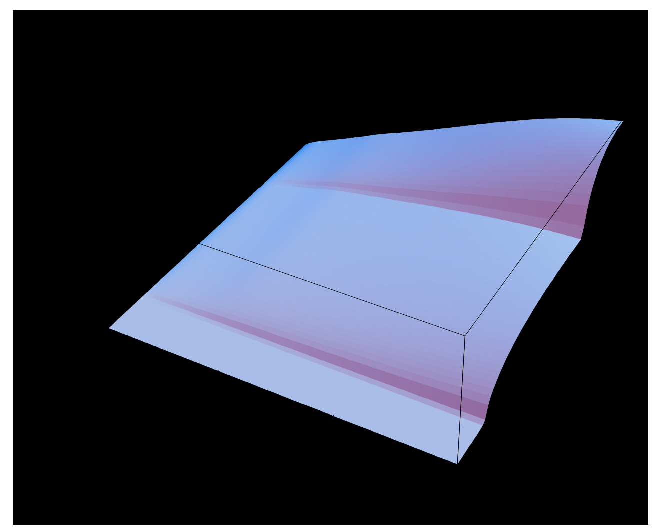
Armchair nanotube

Results

metallic   semiconducting



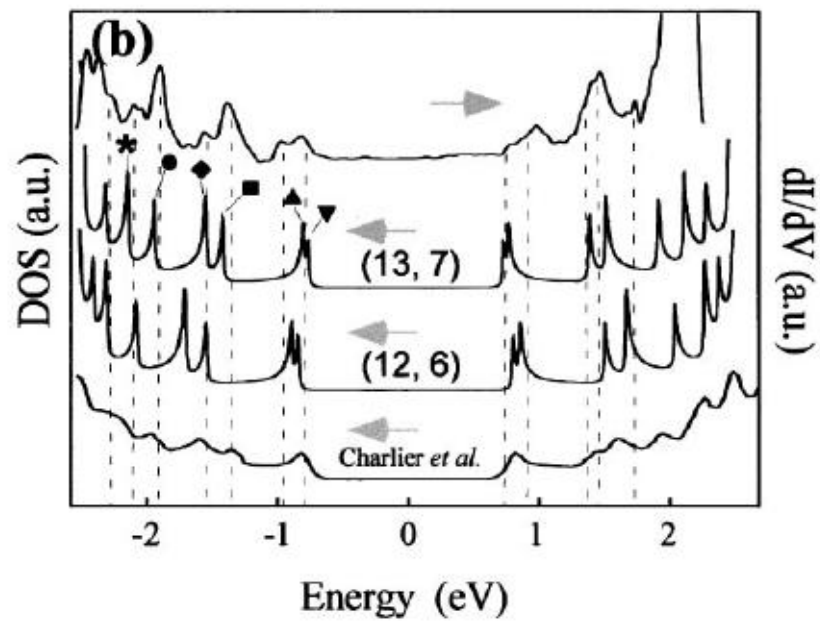




Far from the cap (top), near (middle), in the cap (bottom)

Results, experiment (STM)

- the van Hove singularity (VHS) is smoothed out in DoS
- The amplitude of the peaks grows with z
- At threshold points E=m, the DoS is found to be linear in E-m



P. Kim et al., Phys.Rev.Lett. 82, 1225 (1999): the experimentally observed curve for the metallic nanotube is the upper one

Some open problems (theory)

- Interactions (electron-electron, electron-phonon)
- Disorder (point defects)
- Magnetism
- Multiple layers, 3D graphite
- Etc.