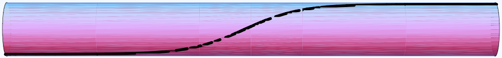
Supersymmetric twisting of carbon nanotubes

Vít Jakubský,
Nuclear Physics Institute, Řež near Prague

Benasque, 12.7. 2012

- Carbon nanotubes: small cyllinders rolled up from graphene sheet.
- What happens if we twist radially the nanotube?
- How will be affected observable quantities (e.g. local density of states)?
- Will there appear bound states?
- Can we construct exactly solvable models to answer these questions?



Dirac electrons in graphene

- tight-binding model

$$\gamma \begin{pmatrix} 0 & h^\dagger(\mathbf{k}) \\ h(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} = E \begin{pmatrix} c_A \\ c_B \end{pmatrix}, \qquad h(\mathbf{k}) = 1 + e^{i\mathbf{k}\mathbf{a_1}} + e^{i\mathbf{k}\mathbf{a_2}}$$

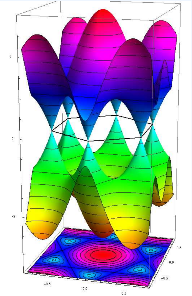
- dispersion relation via tight-binding model (vectors a_i related to the geometry of the crystal)

$$E = \pm\gamma\sqrt{3 + 2\cos \mathbf{k}\mathbf{a_1} + 2\cos \mathbf{k}.\mathbf{a_2} + 2\cos \mathbf{k}(\mathbf{a_2} - \mathbf{a_1})}$$

- six points where $E = 0$, two of them inequivalent, called Dirac points
- in the vicinity of $E = 0$, dispersion relation is linear $E \sim |\mathbf{k}|$
- tight-binding hamiltonian reduces to the first order operator for $E \sim 0$

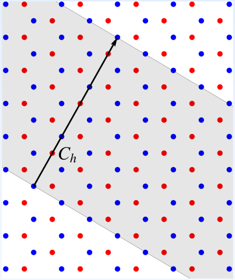
$$h = i\partial_x\sigma_2 + i\partial_y\sigma_1$$

massless Dirac hamiltonian



Carbon nanotubes

- specified by the circumference vector (chiral vector) $\mathbf{C_h}$, it determines its electronic properties



- quantization of momenta associated with the compactified coordinate

$$h = i\sigma_1\partial_x + k_y\sigma_2$$

Deformations as (pseudo-)magnetic field

[Kane, Mele], [Vozmediano]

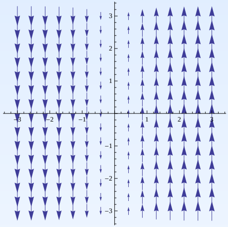
Displacement vector

$$\mathbf{d} = (d_x(x,y), d_y(x,y))$$

Strain tensor

$$s_{xx} = \partial_x d_x, \quad s_{yy} = \partial_y d_y,$$

$$s_{xy} = s_{yx} = \frac{\partial_x d_y + \partial_y d_x}{2}.$$

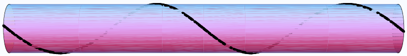


$\mathbf{d} = (0, x)$, $s_{xx} = s_{yy} = 0$, $s_{xy} = 1$

Radially twisted nanotube - $1D$ Dirac Hamiltonian with vector potential

$$h = i\sigma_2\partial_x + \Delta_1(x)\sigma_1$$

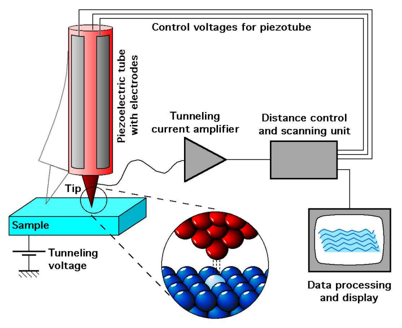
$\Delta_1(x)$ corresponds to the displacement $\mathbf{d} = (0, \int \Delta_1(x)dx)$ of the nanotube



The nanotube with the twist corresponding to $d_y \sim x$. In the untwisted nanotube, the black line would be straight (horizontal).

- Primary objective: solvable models of twisted carbon nanotubes
- Secondary objective:
  - local density of states (LDOS), the quantity measurable in STM
  - Bound-state energies in depedence on the twist

Spectral tunneling microscopy (STM): tunneling current is a function of the position of the tip, voltage and LDOS



STM, figure by Michael Schmid, TU Wien

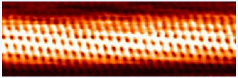


figure by Taner Yildirim, NIST

Darboux transformation L for Dirac Hamiltonians [Samsonov]

Analogy of Witten's construction for $1D$ Dirac Hamiltonian
Initial solvable Hamiltonian $h = i\sigma_2\partial_x + (\Delta_1 + m)\sigma_1$
Transformation L is defined via two eigenvectors $u_{1(2)}$ of h,
$hu_{1(2)} = \lambda_{1(2)} u_{1(2)}$, $\lambda_{1(2)} \in \mathbb{R}$, $Lu_{1(2)} = 0$
We fix $\lambda_1 = -\lambda_2$, $u_1 = (u_{11}, u_{21})^T$, $u_2 = \sigma_3 u_1$

$$L = \mathbf{1}\partial_x - \begin{pmatrix} (\ln u_{11})' & 0 \\ 0 & (\ln u_{22})' \end{pmatrix}, \quad \tilde{h} = i\sigma_2\partial_x - \left(\Delta_1 + m - \lambda_1 \frac{u_{11}^2 + u_{21}^2}{u_{11}u_{21}}\right)\sigma_1.$$

Then

$$\tilde{h}L = Lh$$

- h and $\tilde{h}$ are spectrally almost identical (assuming regular DT)
- possible difference: $\tilde{h}$ can have to two additional bound states with energy $E = \pm\lambda_1$

Eigenstates of $\tilde{h}$ corresponding to $\lambda_k \neq \pm\lambda_1$,

$$\tilde{\phi}_k = \frac{L\phi_k}{\sqrt{(\lambda_k - \lambda_1)(\lambda_k - \lambda_2)}}, \quad \tilde{h}\tilde{\phi}_k = \lambda_k\tilde{\phi}_k.$$

Green's function and LDOS for the twisted nanotubes

Green's function for the initial system

$$(h-\lambda)G(x,y;\lambda)=\delta(x-y),\quad \lambda\in\mathbb{C}.$$

$$G(x,y;\lambda)=\frac{\psi_\lambda(x)\xi_\lambda(y)^T\theta(x-y)+\xi_\lambda(x)\psi_\lambda(y)^T\theta(y-x)}{W(\psi_\lambda,\xi_\lambda)},$$

where $h\psi_\lambda=\lambda\psi_\lambda$, $h\xi_\lambda=\lambda\xi_\lambda$ for any $\lambda\in\mathbb{C}$. Wronskian
$W(\psi,\xi)=i\psi(x)^T\sigma_2\xi(x),\quad \partial_x W(\psi_\lambda,\xi_\lambda)=0$
Green's function for the new Hamiltonian $\tilde{h}$

$$\tilde{G}(x,y;\lambda)\quad=\quad\frac{\tilde{\psi}_\lambda(x)\tilde{\xi}_\lambda(y)^T\theta(x-y)+\tilde{\xi}_\lambda(x)\tilde{\psi}_\lambda(y)^T\theta(y-x)}{W(\tilde{\psi}_\lambda,\tilde{\xi}_\lambda)}$$

where $\lambda\neq\pm\lambda_1$ and $\tilde{h}\tilde{\psi}_\lambda=\lambda\tilde{\psi}_\lambda,\quad \tilde{h}\tilde{\xi}_\lambda=\lambda\tilde{\xi}_\lambda,$

$$\tilde{\psi}_\lambda=\frac{L\psi_\lambda}{\sqrt{(\lambda-\lambda_1)(\lambda-\lambda_2)}},\quad \tilde{\xi}_\lambda=\frac{L\xi_\lambda}{\sqrt{(\lambda-\lambda_1)(\lambda-\lambda_2)}}$$

Note: Wronskian satisfies $W(\tilde{\psi},\tilde{\xi})=W(\psi,\xi)$

Green's function part II

The action of L on the eigenstates ψ of h can be simplified

$$\tilde{\psi}_\lambda = \frac{L\psi}{\sqrt{(\lambda-\lambda_1)(\lambda-\lambda_2)}} = \mathcal{L}(\lambda,x)\psi_\lambda, \quad \mathcal{L}(\lambda,x) = -i\sigma_2 \frac{\lambda - U(x)\Lambda U^{-1}(x)}{\sqrt{(\lambda-\lambda_1)(\lambda-\lambda_2)}},$$

where $\Lambda = diag(\lambda_1, \lambda_2)$.
Green's function $\tilde{G}(x,y;\lambda)$ is then

$$\tilde{G}(x,y;\lambda) = \mathcal{L}(\lambda,x)G(x,y;\lambda)\mathcal{L}^T(\lambda,y).$$

It can be computed by **purely algebraic means** from $G(x,y;\lambda)$!
LDOS for carbon nanotubes

$$\tilde{\rho}(x,\lambda) = -\frac{1}{\pi}\lim_{\mathrm{Im}\lambda\to 0_+} \mathrm{Im}\, Tr\, \tilde{G}(x,x;\lambda).$$

It can be written as

$$\tilde{\rho}(x,\lambda) = -\frac{1}{\pi}\lim_{\mathrm{Im}\lambda\to 0_+} \mathrm{Im}\, Tr\left(\mathcal{L}(\lambda,x)^T\mathcal{L}(\lambda,x)\, G(x,x;\lambda)\right).$$

The trace of $\tilde{G}(x, x; \lambda)$ is

$$\begin{aligned} \mathrm{Tr}(\tilde{G}(x,x;\lambda)) &= g_0 + \frac{2\lambda_1^2 g_0 (u_1^\dagger u_1)^2}{(\lambda^2 - \lambda_1^2)(\det U_{II})^2} \\ &+ \frac{2\lambda_1^2 u_1^\dagger u_1}{(\lambda^2 - \lambda_1^2)(\det U)^2} \left(-g_3 u_1^\dagger \sigma_3 u_1 - g_1 \frac{\lambda}{\lambda_1} u_1^\dagger \sigma_1 u_1 \right). \end{aligned}$$

where $g_j = \mathrm{Tr}(\sigma_j G(x, x; \lambda))$ for $j = 0, .., 3$, $\sigma_0 = \mathbf{1}$.

Double-kink model

Initial (free-particle) and the new Hamiltonians

$$h = i\sigma_2\partial_x + m\sigma_1, \quad \tilde{h} = i\sigma_2\partial_x + (m - k\tanh kx + k\tanh(kx+a))\sigma_1.$$

The kernel of L consists of u_1, $u_2 = \sigma_3 u_1$, $hu_{1(2)} = \pm\lambda_1 u_{1(2)}$

$$u_1 = (\frac{1}{\sqrt{k}}\cosh kx, \frac{1}{\sqrt{k}}\cosh(kx+a))^T$$

where $a = \frac{1}{2}\log\frac{m-k}{m+k}, \quad k = \sqrt{m^2 - \lambda_1^2}, \quad 0 < \lambda_1 < m.$
$\tilde{h}$ has two bound states v_1 and v_2,

$$v_1 = \frac{\sqrt{k}}{2}(\operatorname{sech} kx, \operatorname{sech}(kx+a))^T, \quad v_2 = \sigma_3 v_1 = \frac{\sqrt{k}}{2}(\operatorname{sech} kx, -\operatorname{sech}(kx+a))^T.$$

The LDOS can be rewritten again in terms of LDOS of the free system ρ and the probability density of the bound states

$$\tilde{\rho}(x,\lambda) = \rho(x,\lambda)\left(1 - \frac{2\,k\,v_1^\dagger v_1}{(\lambda^2 - \lambda_1^2)}\right),$$

Interpretation of the model

External constant magnetic flux $\tilde{\Delta}_{MG} = m$ parallel with the axis of the nanotube
The twisting part of the potential
$\tilde{\Delta}_T = -k \tanh kx + k \tanh(kx + a) \rightarrow$ asymptotically vanishing twist localized mainly at the origin

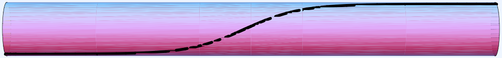


Figure: The nanotube associated with the Hamiltonian $\tilde{h}$ and the twist corresponding to $d_y \sim \ln \frac{\cosh(kx+a)}{\cosh kx}$. The constant part of the magnetic field in $\tilde{h}$ can be attributed to the external magnetic field or to the semi-conducting character of the nanotube.

Bound states in dependence on the asymptotic twist

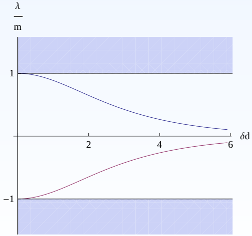
- deformation

$$d_y \sim \ln \frac{\cosh(kx+a)}{\cosh kx}, \quad k = \sqrt{m^2 - \lambda_1^2}$$

- asymptotic twist in dependence on the bound states

$$\delta d = \left| \lim_{x\to\infty} d_y - \lim_{x\to-\infty} d_y \right| = 2|a| = -\ln \frac{m - \sqrt{m^2-\lambda_1^2}}{m + \sqrt{m^2-\lambda_1^2}}.$$

Energies in dependence on the asymptotic twist



$$\lambda_1 = \pm 2m \frac{e^{\frac{\delta d}{2}}}{1+e^{\delta d}}$$

Summary and Outlook

- the formulas for $\tilde{G}(x, y, \lambda)$ hold for quite general class of seed Hamiltonians
- the operator $h = i\sigma_2\partial_x + \Delta_1\sigma_1$ appears in the context of
  - (1+1)dimensional Nambu-Jona-Lasinio (chiral Gross-Neveu) model
  - in the analysis of inhomogeneous superconductors
  - in describtion of vortex in the extreme type-II superconductors
  - describes fermions coupled to solitons in the linear molecules (polyacetylene)

References:

[1] L. M. Nieto, A. A. Pecheritsin, and B. F. Samsonov, Annals Phys. 305, 151 (2003).
[2] C. L. Kane, E. J. Mele, Phys. Rev. Lett. 78, 1932 (1997).
[3] M. A. H. Vozmediano, M. I. Katsnelson and F. Guinea, Phys. Rept. 496, 109 (2010).
[4] V. Jakubský, M. P. Plyushchay, Phys. Rev. D85, 045035, (2012).