Carbon nanotubes: Models, correlations and the local density of states

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in collaboration with

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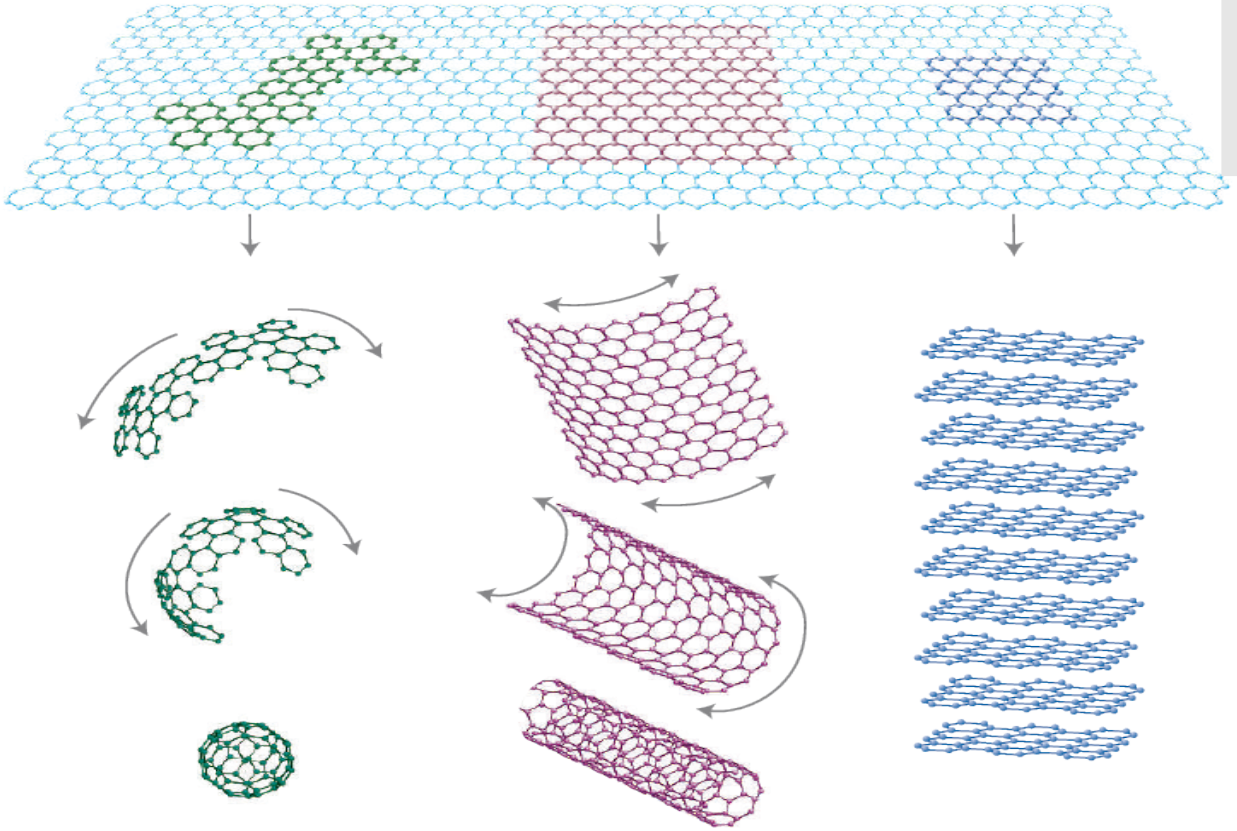
Condensed matter systems with variable many-body interactions

Outline

- Carbon structures
- Modelling of a carbon nanotube
- Effective ladder model
- Correlations in a carbon nanotube and the local density of states

Carbon structures



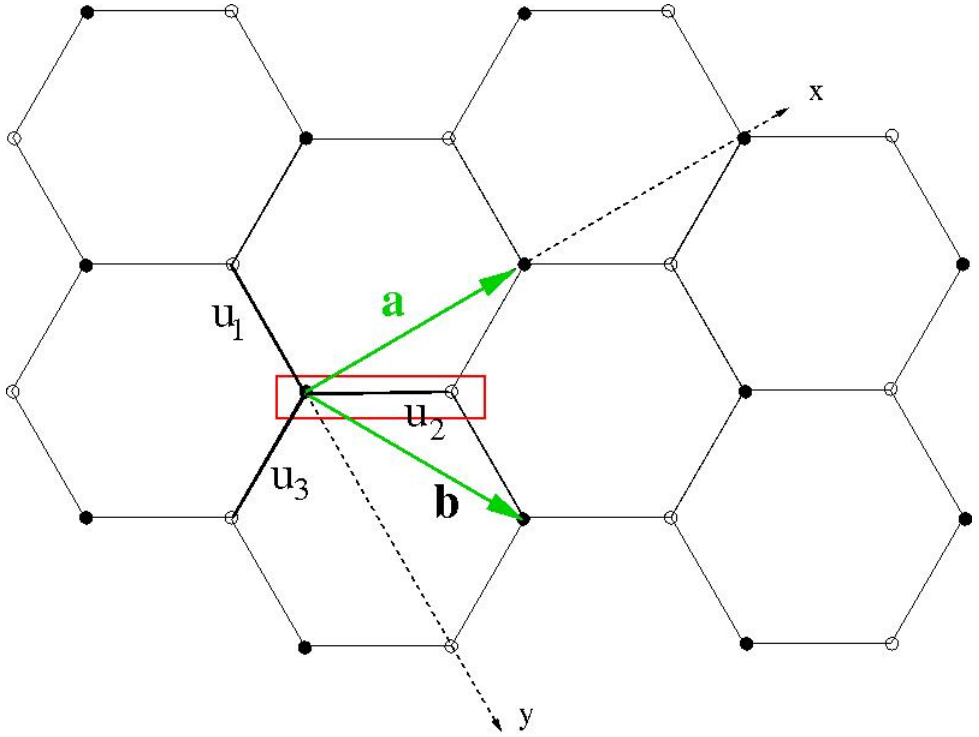
"Graphene": 2D carbon layer (planar, sp2 hybridization in chemical bond

0D: Fullerene

1D: Carbon nanotube

3D: Graphite

Graphene: electronic properties



Lattice with 2-atom basis

$$\mathbf{a} = \sqrt{3}a\ (1,0) \qquad \mathbf{b} = \sqrt{3}a\ (\frac{1}{2}, \frac{\sqrt{3}}{2})$$

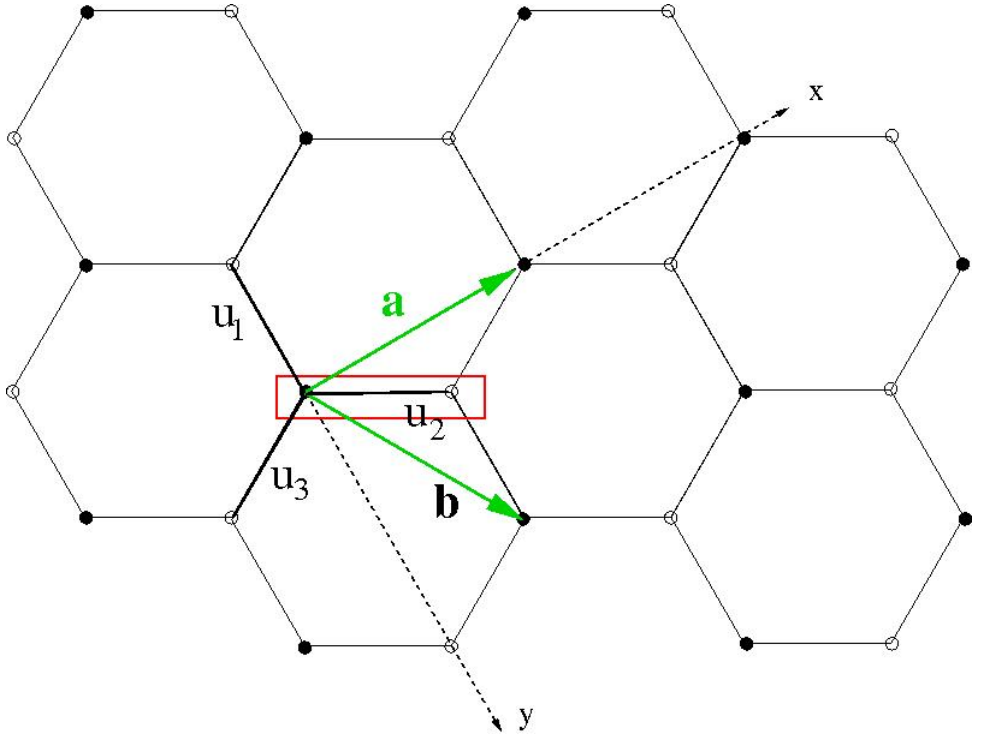
reciprocal lattice vectors

$$\mathbf{k}_1 = \frac{2\pi}{\sqrt{3}a}\ (1, -\frac{1}{\sqrt{3}}) \qquad \mathbf{k}_2 = \frac{4\pi}{3}\ (0,1)$$

Hamiltonian (nearest neighbour hopping)

$$H = -t \sum_{<ij>} c_i^\dagger c_j + c_j^\dagger c_i$$

Graphene: electronic properties



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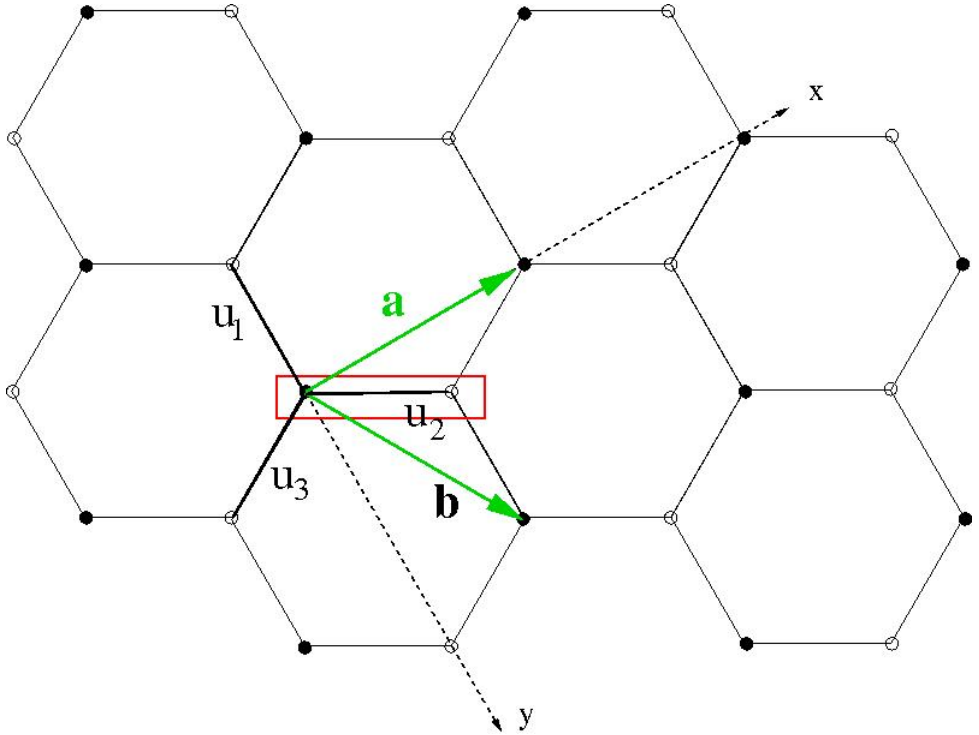
Stationary states: $$\psi^\dagger = \sum_{i,\bullet} A_\bullet\ e^{\imath \mathbf{k}\cdot\mathbf{r}_i} c_i^\dagger + \sum_{i,\circ} A_\circ\ e^{\imath \mathbf{k}\cdot\mathbf{r}_i} c_i^\dagger$$

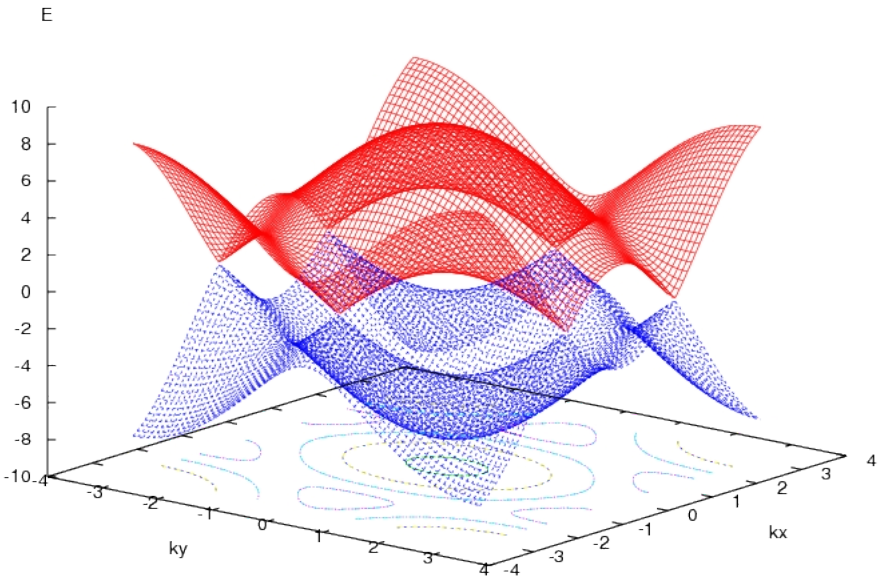
if $$\begin{pmatrix} 0 & -t\sum_{j=1}^{3} e^{\imath \mathbf{k}\cdot\mathbf{u}_j} \\ -t\sum_{j=1}^{3} e^{\imath \mathbf{k}\cdot\mathbf{v}_j} & 0 \end{pmatrix} \begin{pmatrix} A_\bullet \\ A_\circ \end{pmatrix} = \epsilon_k \begin{pmatrix} A_\bullet \\ A_\circ \end{pmatrix}$$

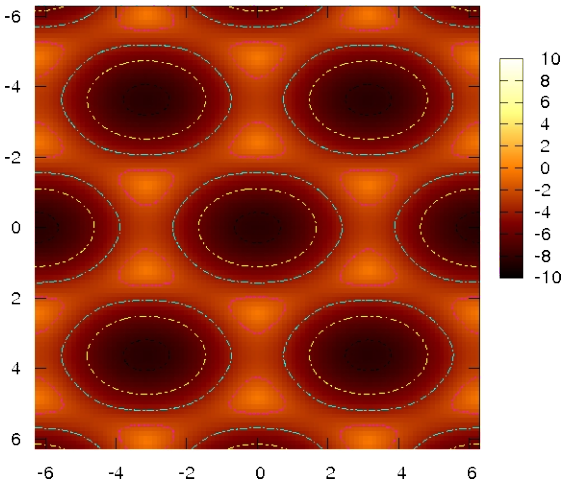
Graphene: electronic properties



Dispersion

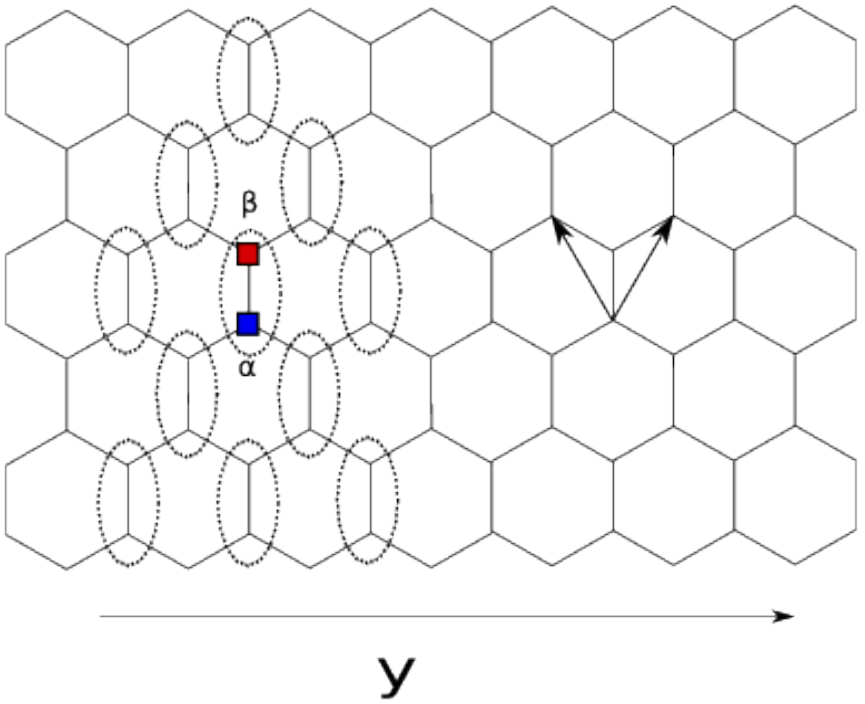
$$\epsilon_{\mathrm{k}} = \pm\sqrt{1 + 4\cos^2(\frac{\sqrt{3}}{2}k_x) + 4\cos(\frac{\sqrt{3}}{2}k_x)\cos(\frac{3}{2}k_y)}$$





6 „Fermi points“, 2 independent

From graphene to CNT



Wrap the sheet around

"Roll-up" vector

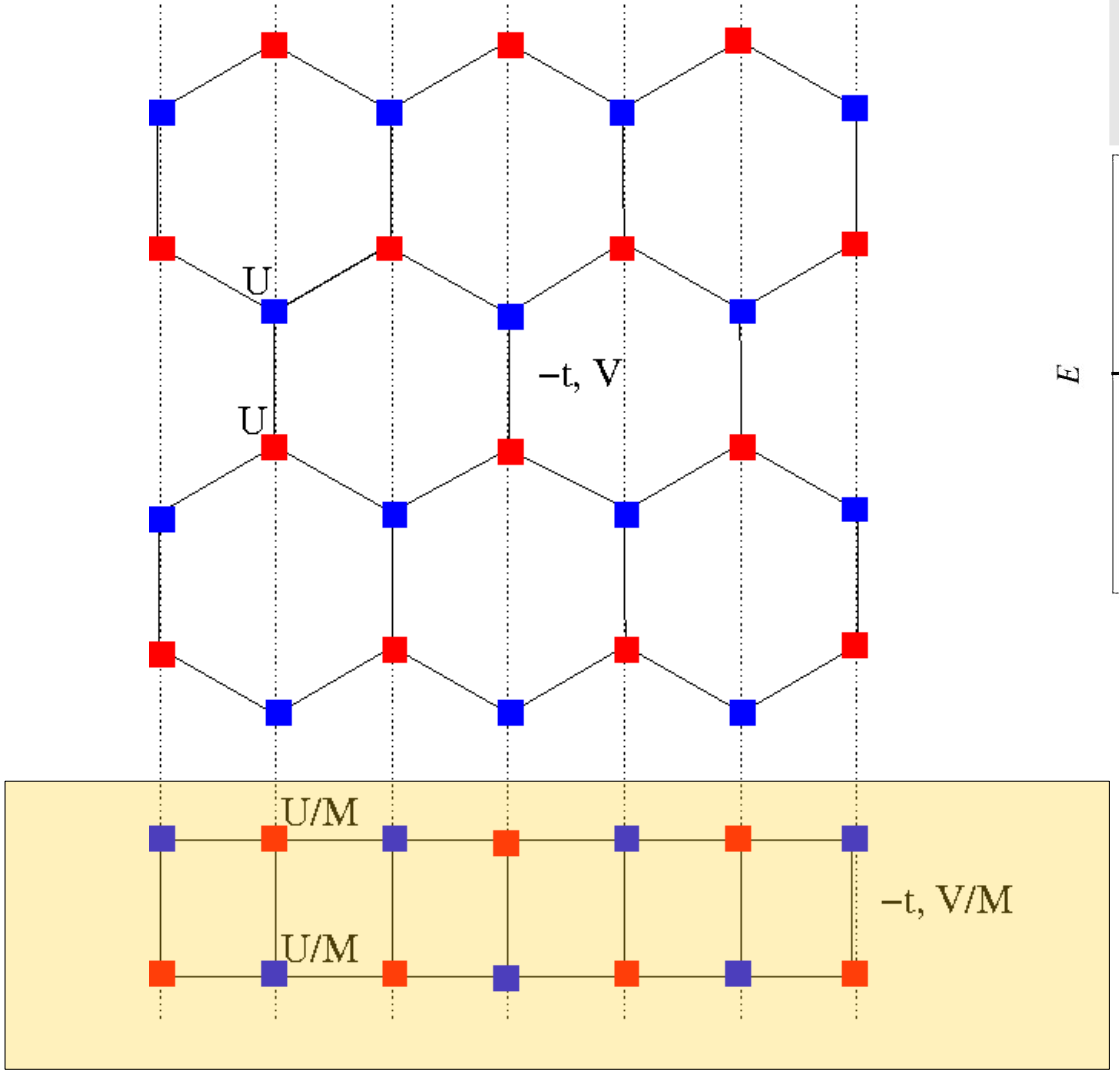
$$\vec{c} = n_1 \, \vec{e}_1 + n_2 \, \vec{e}_2$$

Periodic boundary conditions at the seam !

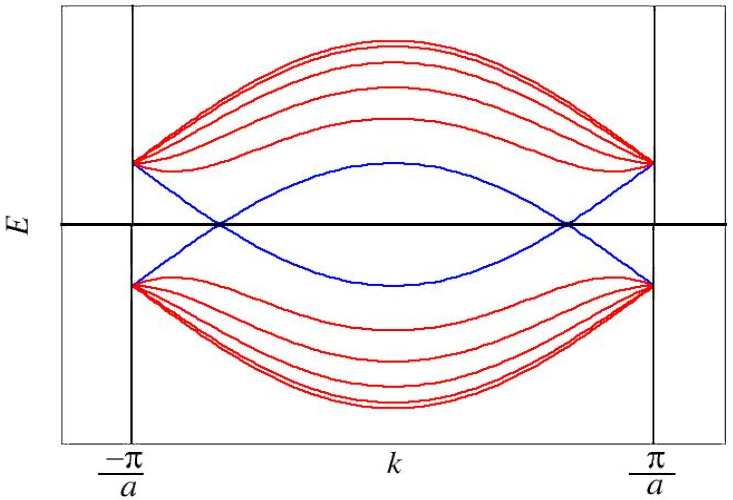
Armchair CNT

$n_1 = -n_2$ Zigzag CNT

Armchair CNT: minimal model



New band structure: only one free momentum *k,* the other is fixed to discrete modes from pbc

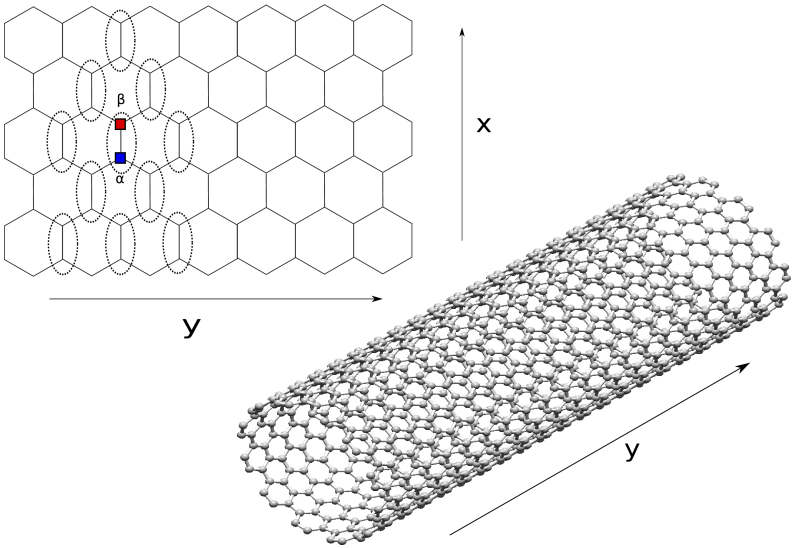


Keep only two bands:

Two-species extended Hubbard model

Solve with DMRG

Armchair CNT with interactions



Tight binding description

$$H = H_0 + H_{\text{int}}$$

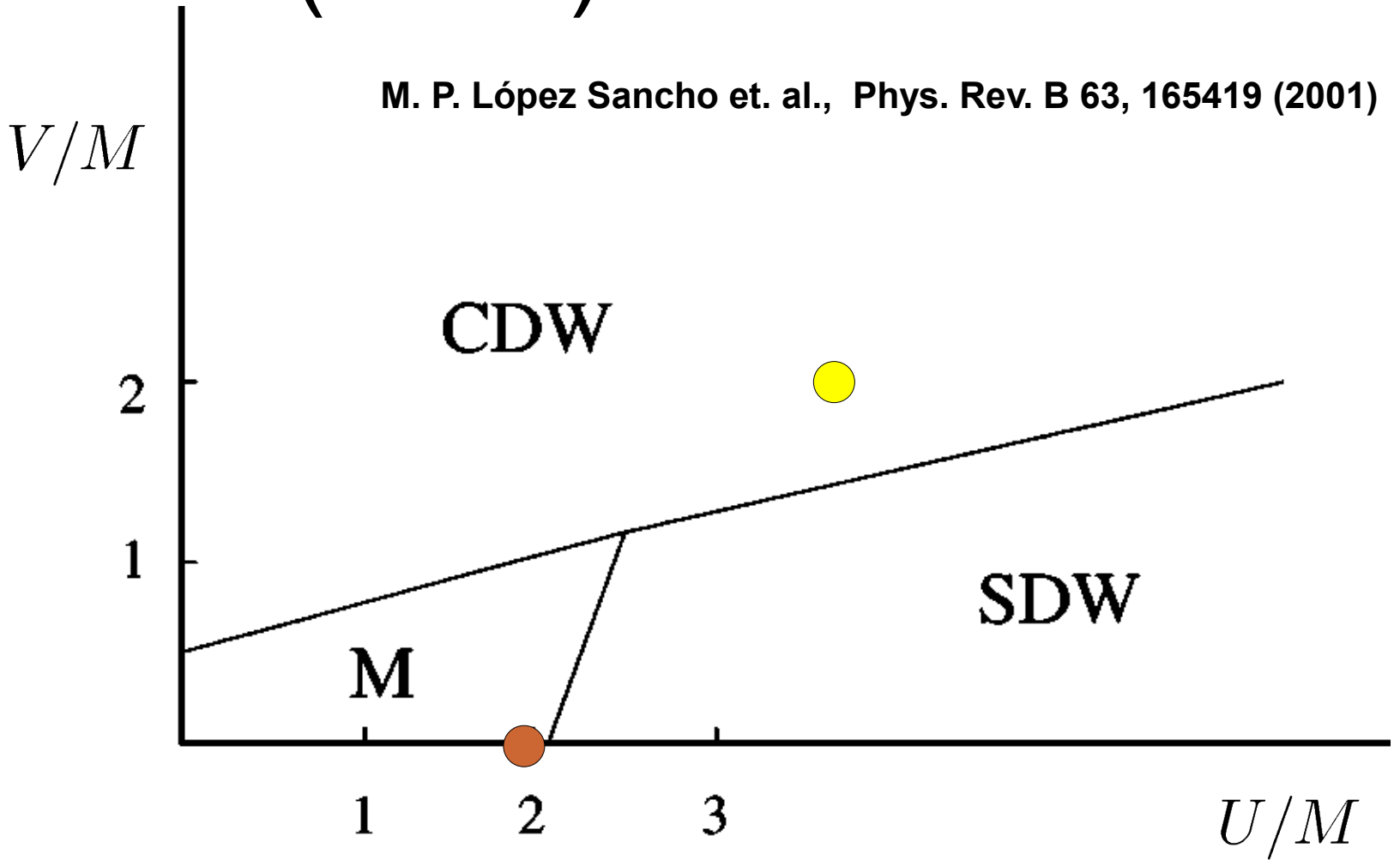
$$H_0 = -t \sum_{\sigma} \sum_{x=1}^{N} \left\{ \sum_{\text{y odd}} \alpha_{xy}^{\sigma\dagger} \beta_{xy+1}^{\sigma} + \beta_{xy}^{\sigma\dagger} \alpha_{x+1y+1}^{\sigma} + \sum_{\text{y even}} \beta_{xy}^{\sigma\dagger} \alpha_{xy+1}^{\sigma} + \alpha_{xy}^{\sigma\dagger} \beta_{x-1y+1}^{\sigma} + \sum_{y=1}^{L} \alpha_{xy}^{\sigma\dagger} \beta_{xy}^{\sigma} + \text{h.c.} \right\}$$

$$H_{\text{int}} = U \sum_{\text{x,y odd}} n_{\alpha}^{\uparrow}(x,y) n_{\alpha}^{\downarrow}(x,y) + U \sum_{\text{x,y even}} n_{\beta}^{\uparrow}(x,y) n_{\beta}^{\downarrow}(x,y)$$

$$+ V \sum_{\sigma,\sigma'} \sum_{x,y} \left\{ n_{\alpha}^{\sigma}(x,y) n_{\beta}^{\sigma'}(x,y) + n_{\alpha}^{\sigma}(x,y) n_{\beta}^{\sigma'}(x,y+1) + n_{\alpha}^{\sigma}(x,y) n_{\beta}^{\sigma'}(x+1,y+1) \right\}$$

Mean field phase diagram of a (clean) armchair CNT

M. P. López Sancho et. al., Phys. Rev. B 63, 165419 (2001)



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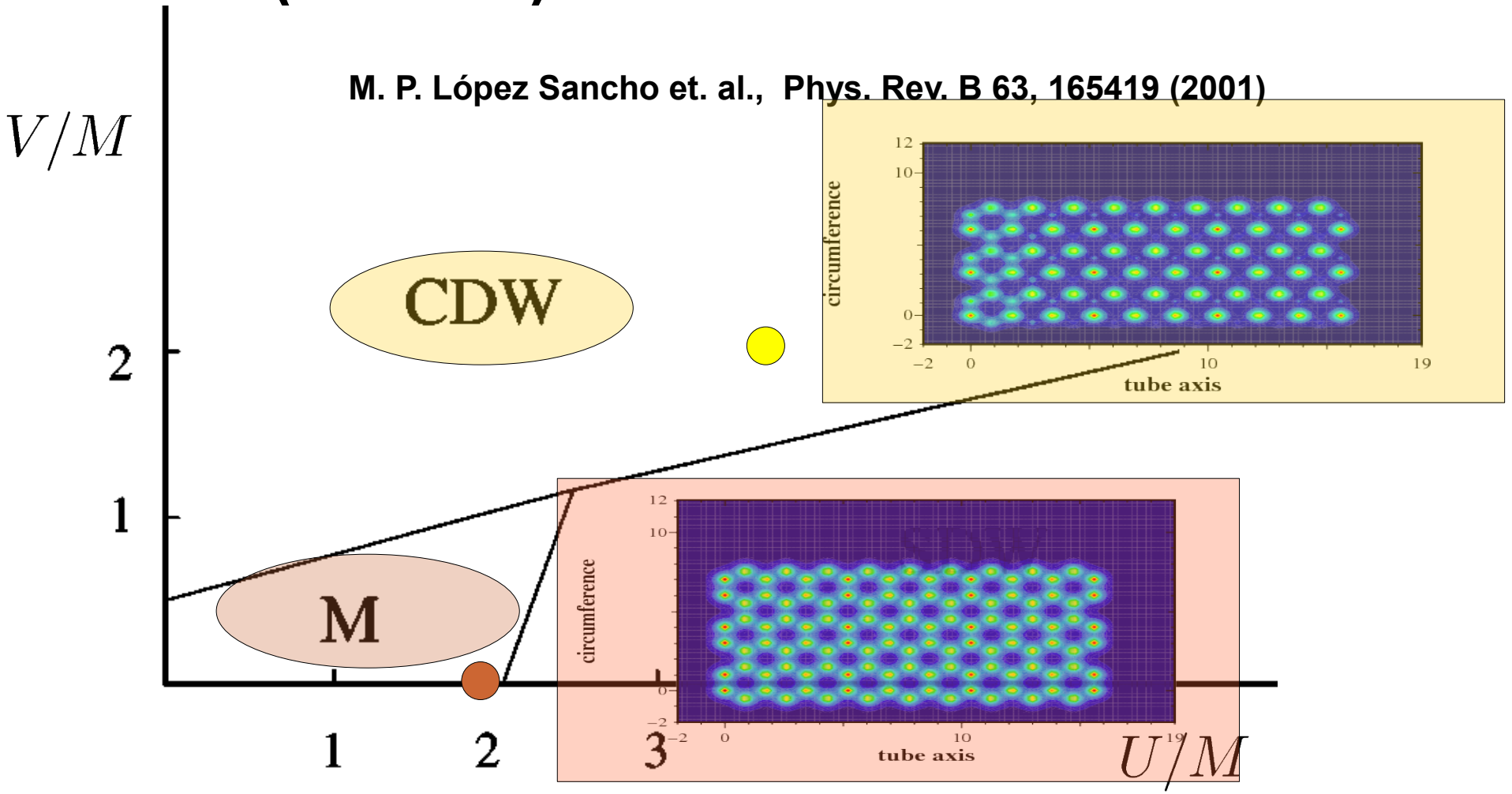

Detecting interactions: The local density of states

$$\rho(x,\omega) = \sum_m |\langle \omega_m; N+1|\psi^\dagger(x)|\omega_0; N\rangle|^2 \delta\left(\omega - (\omega_m - \omega_0)\right)$$

Central quantity in STM measurements
Direct indicator for electron-electron interactions
“Quantifier” for Luttinger liquid behaviour

I. Schneider, A.Struck, M.Bortz, S.Eggert, Phys. Rev. Lett. 101,206401 (2008)

I. Schneider, S.Eggert, Phys. Rev. Lett. (2010)

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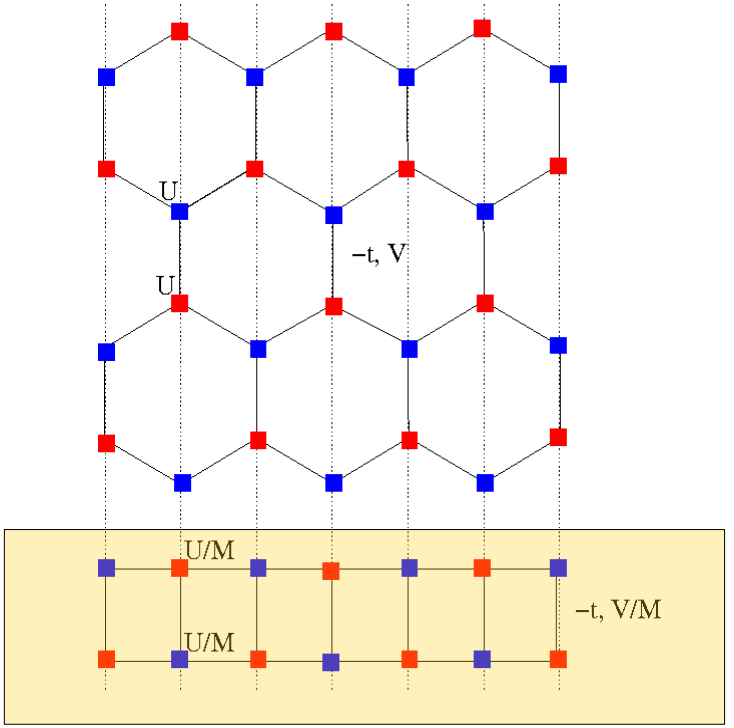
In carbon nanotubes

$$\psi^\dagger(x) = \sum_i \sum_\gamma \phi(x - x_\gamma)\gamma_i^\dagger$$

$$\gamma_i^\dagger = \alpha_i^\dagger,\ \beta_i^\dagger$$



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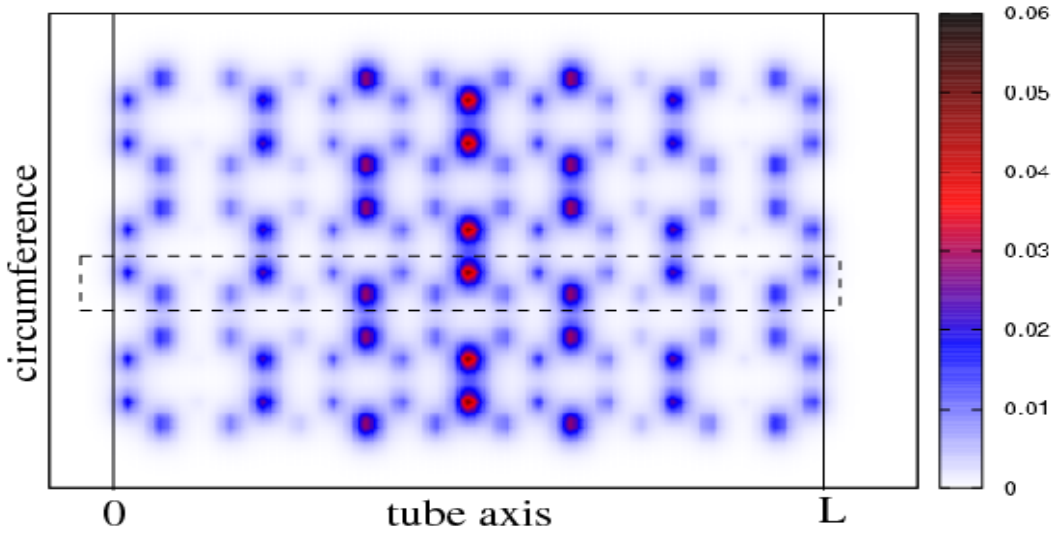

(remapped to carbon lattice)

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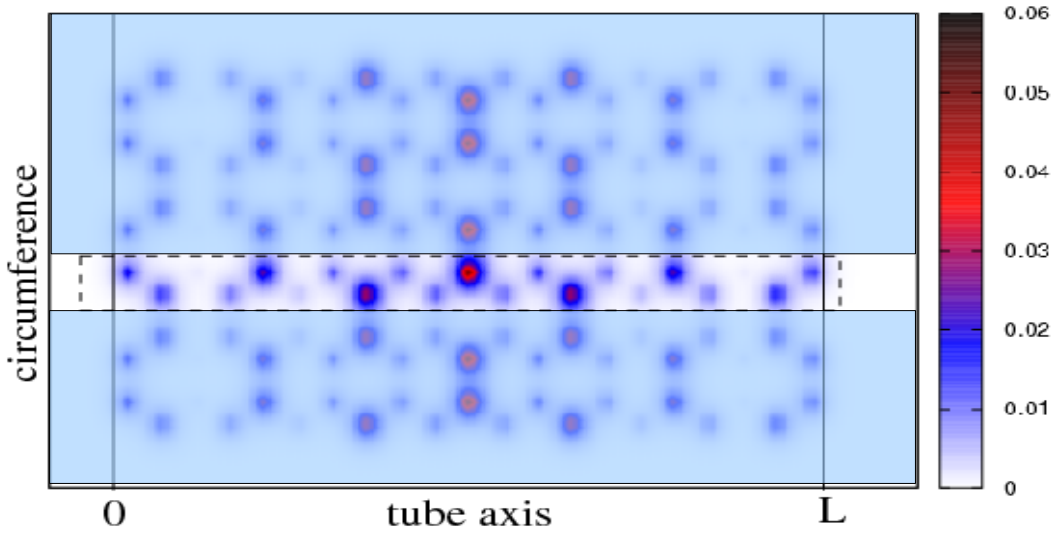

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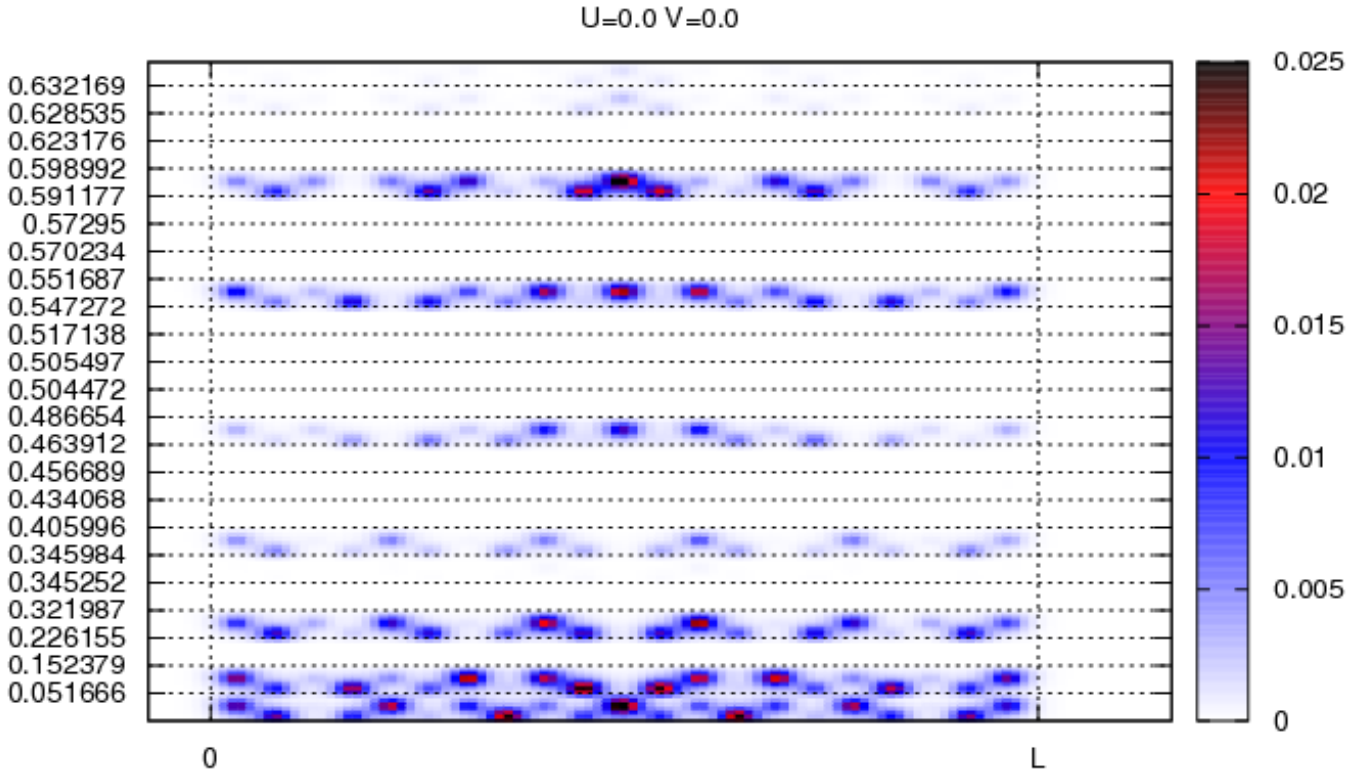
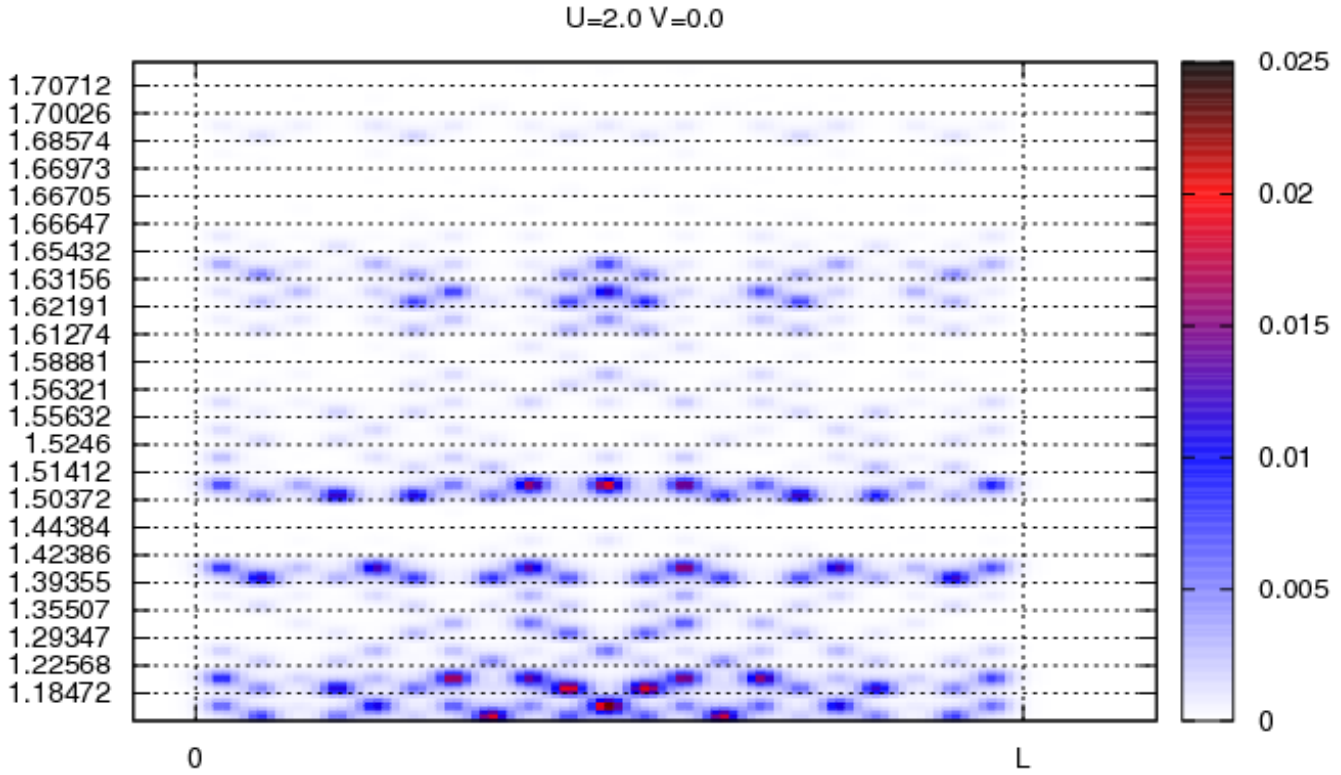
Spectral resolution of LDOS



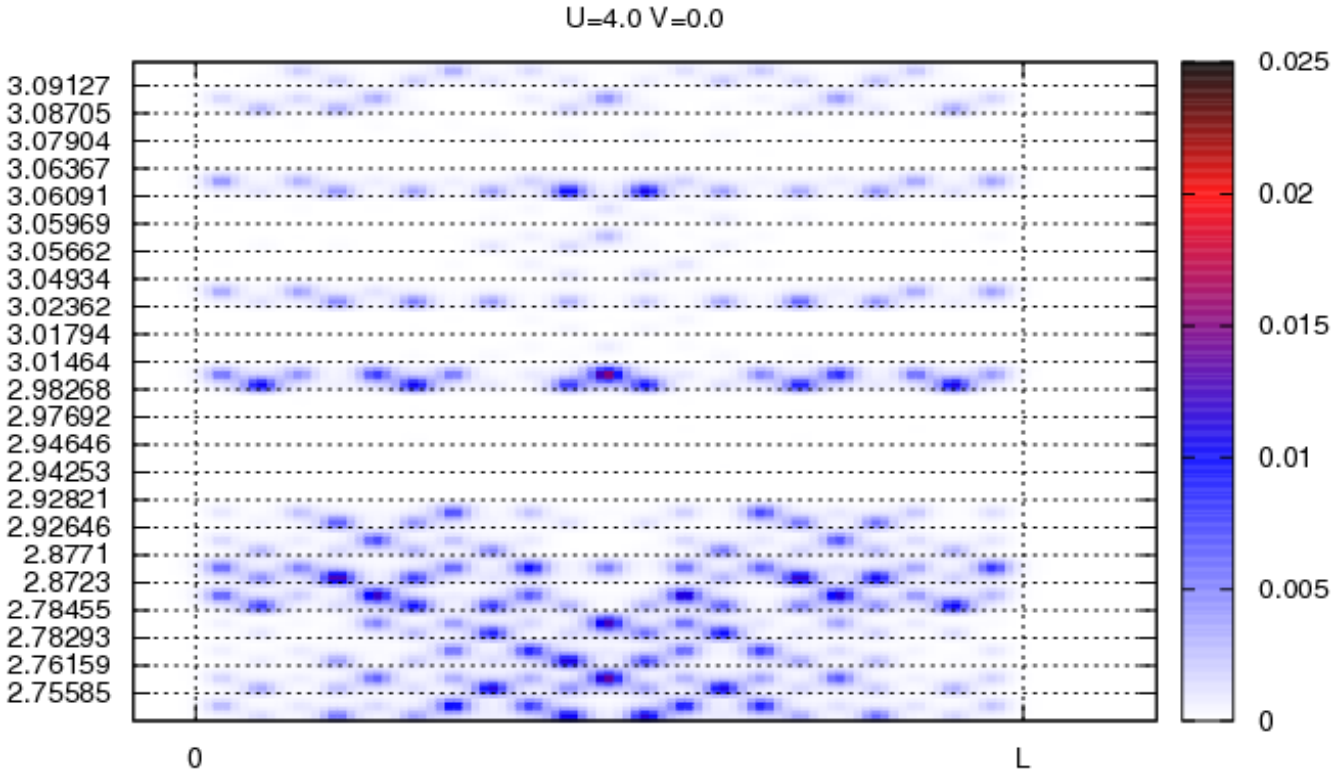
$$\frac{U}{M} = 0, \quad \frac{V}{M} = 0$$

Spectral resolution of LDOS



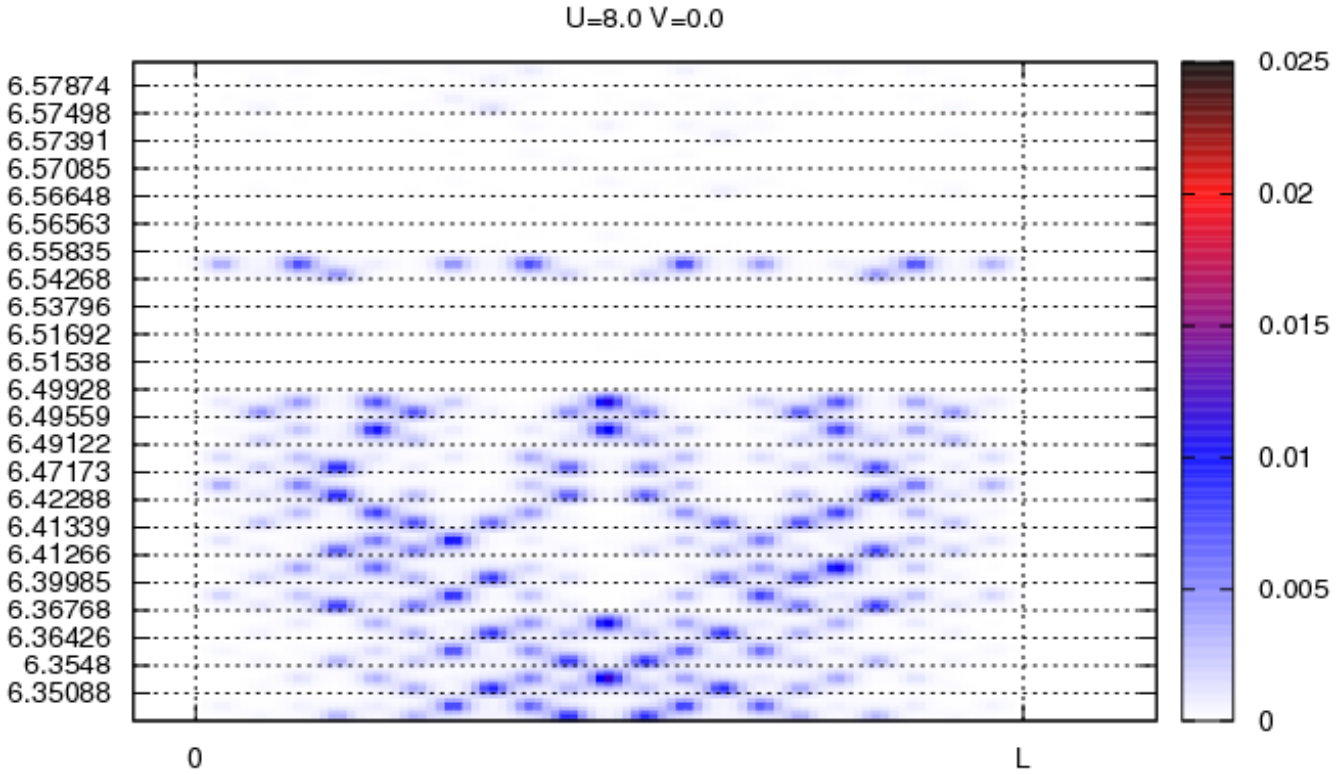
$$\frac{U}{M} = 2, \quad \frac{V}{M} = 0$$

Spectral resolution of LDOS



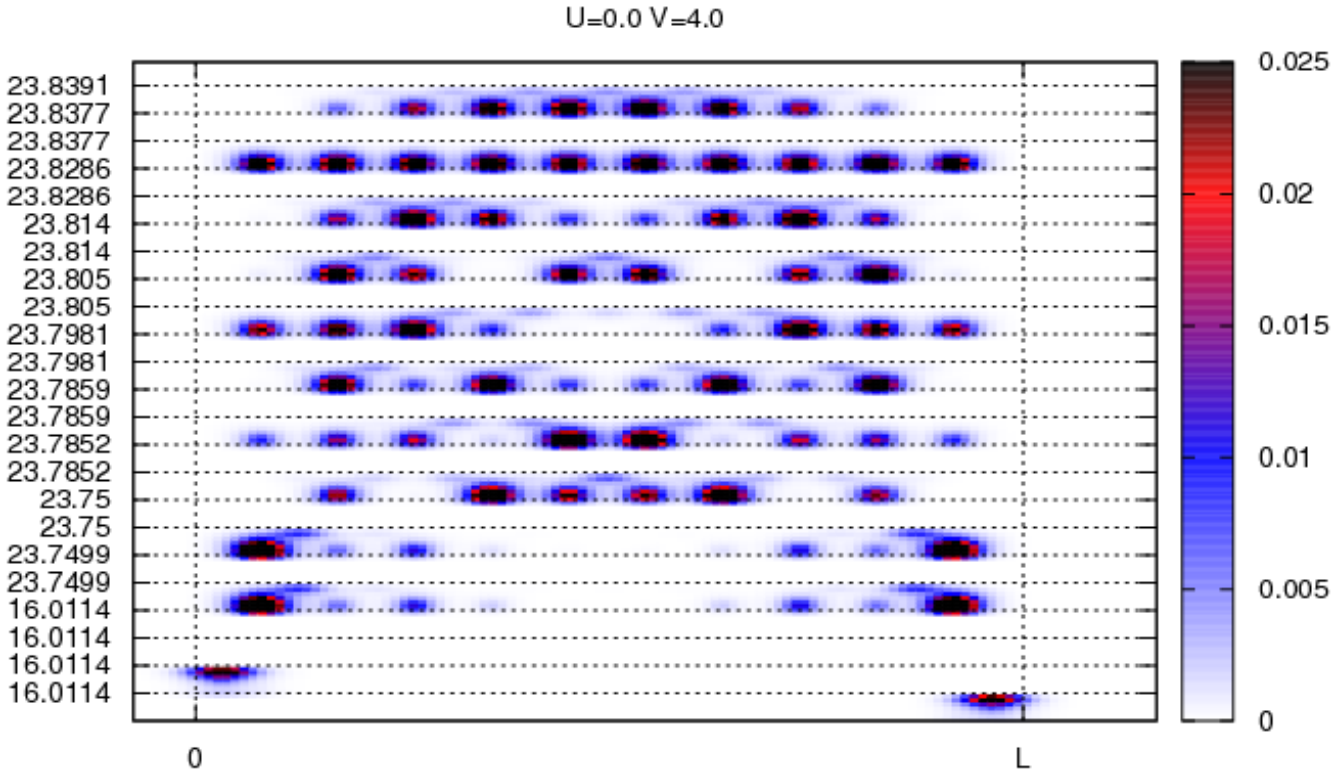
$$\frac{U}{M} = 4, \quad \frac{V}{M} = 0$$

Spectral resolution of LDOS



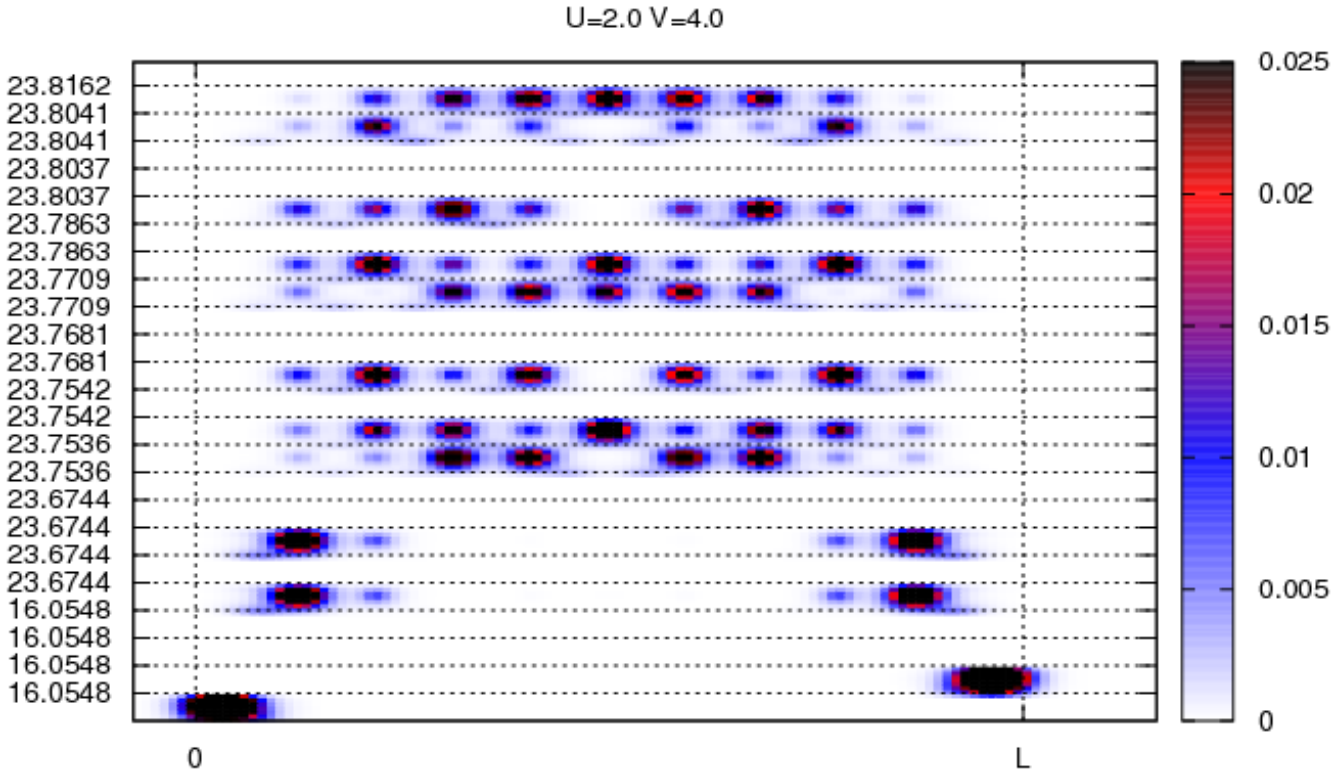
$$\frac{U}{M} = 8, \quad \frac{V}{M} = 0$$

Spectral resolution of LDOS



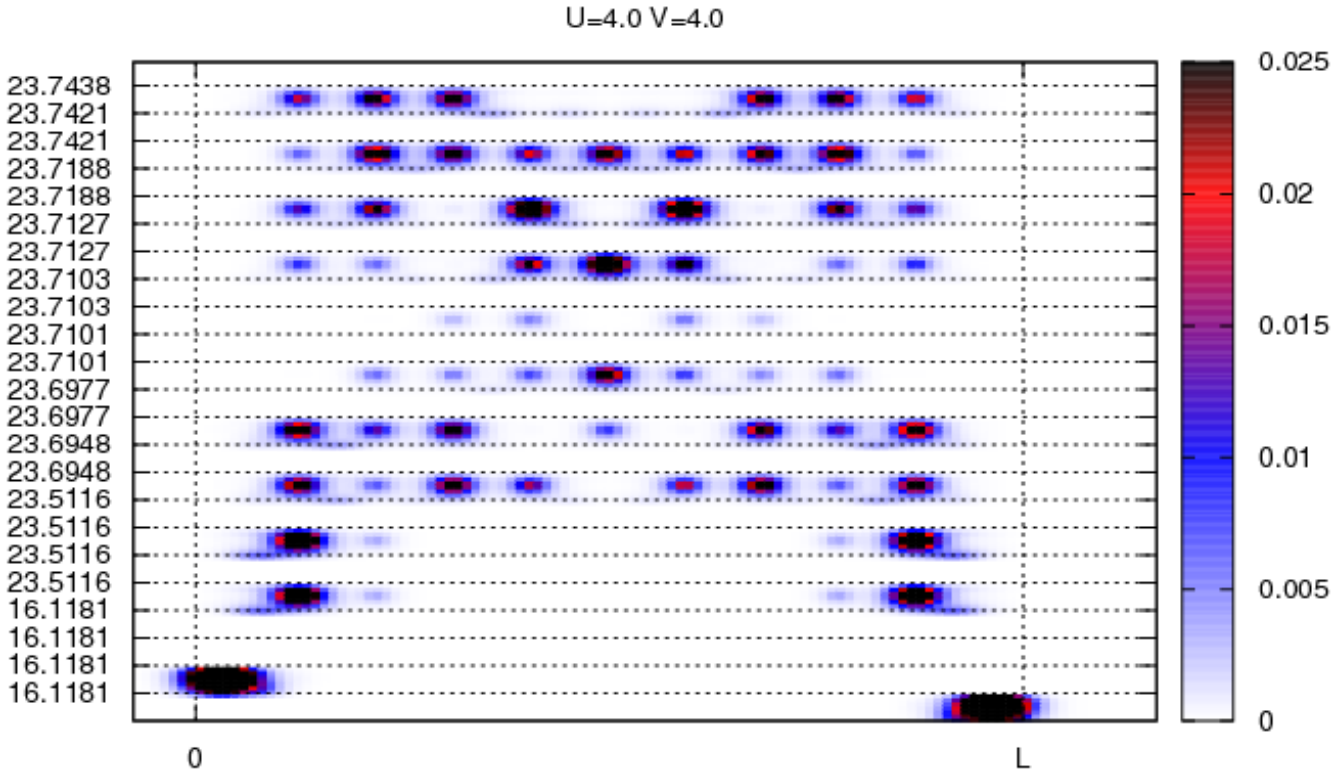
$$\frac{U}{M} = 0, \quad \frac{V}{M} = 4$$

Spectral resolution of LDOS



$$\frac{U}{M} = 2, \quad \frac{V}{M} = 4$$

Spectral resolution of LDOS



$$\frac{U}{M} = 4, \quad \frac{V}{M} = 4$$

Conclusion

Effective Hubbard ladder models allow for DMRG studies of LDOS spectra in carbon nanotubes

LDOS patterns strongly indicate electron interactions in the nanotube

Literature:

S.A.Reyes, A. Struck, S. Eggert, Lattice defects and boundaries in conducting carbon nanotubes, **Phys. Rev. B 80, 075115 (2009)**

I. Schneider, A.Struck, M.Bortz, S.Eggert, Local density of states for finite quantum wires, **Phys. Rev. Lett. 101,206401 (2008)**