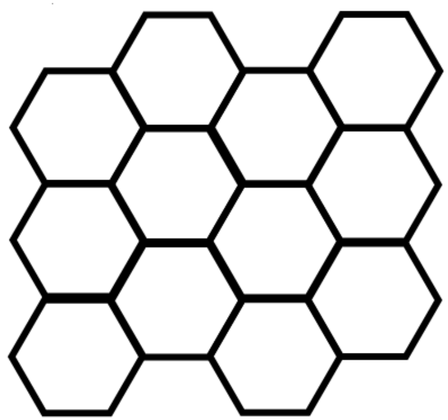
TORQUE GENERATION BY ELECTRIC CURRENT IN (n,1) NANOTUBES

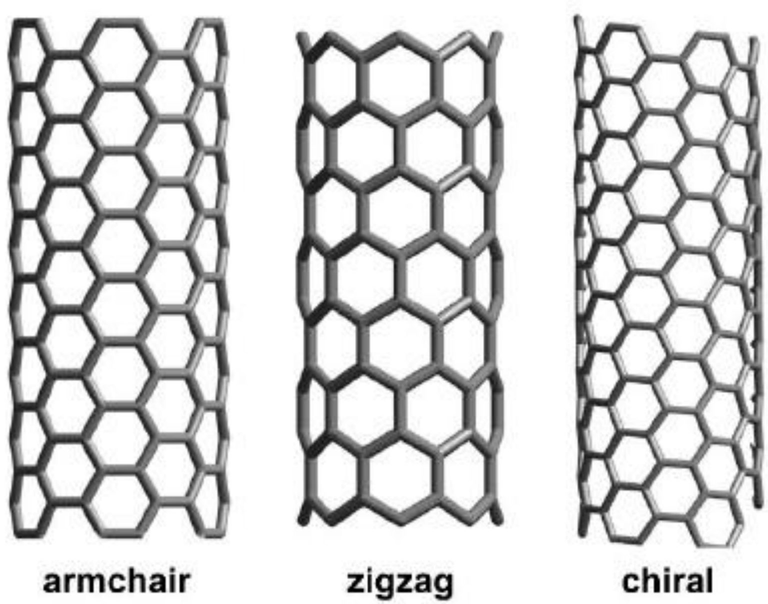
Spiros Evangelou and Shi-Jie Xiong



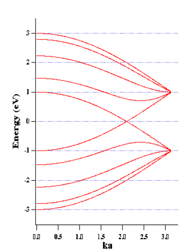
graphene: a sheet of carbon atoms on a hexagonal lattice (the same as other 2D?)

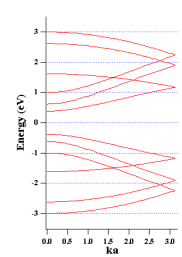
carbon nanotubes (n,m)

rolled-up graphene into long wires



(n,n) (n,0) (n,m)





n-m=3k → metallic

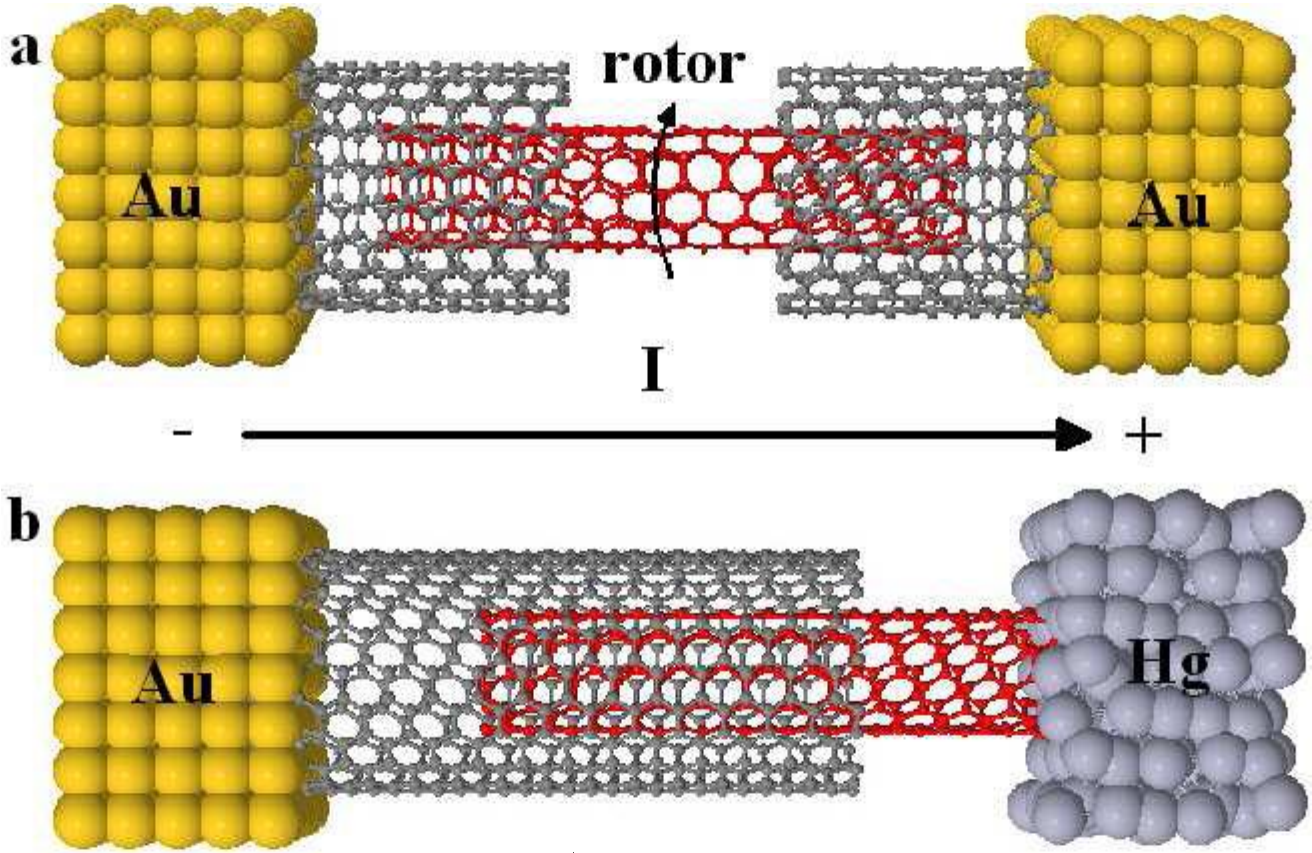
helicity: m helical lines (superlattice structures)

high-purity

- ✓ **nano-devices** (electron and spin based) alternative to conventional wires for quantum info and spintronics
- ✓ **helicity** as in proteins, DNA, ... **strong spin-orbit** coupling, etc.
- ✓ **gap** can appear via external fields and mechanical deformations
- ✓ **ballistic** transport

nanomotor (NEMS)

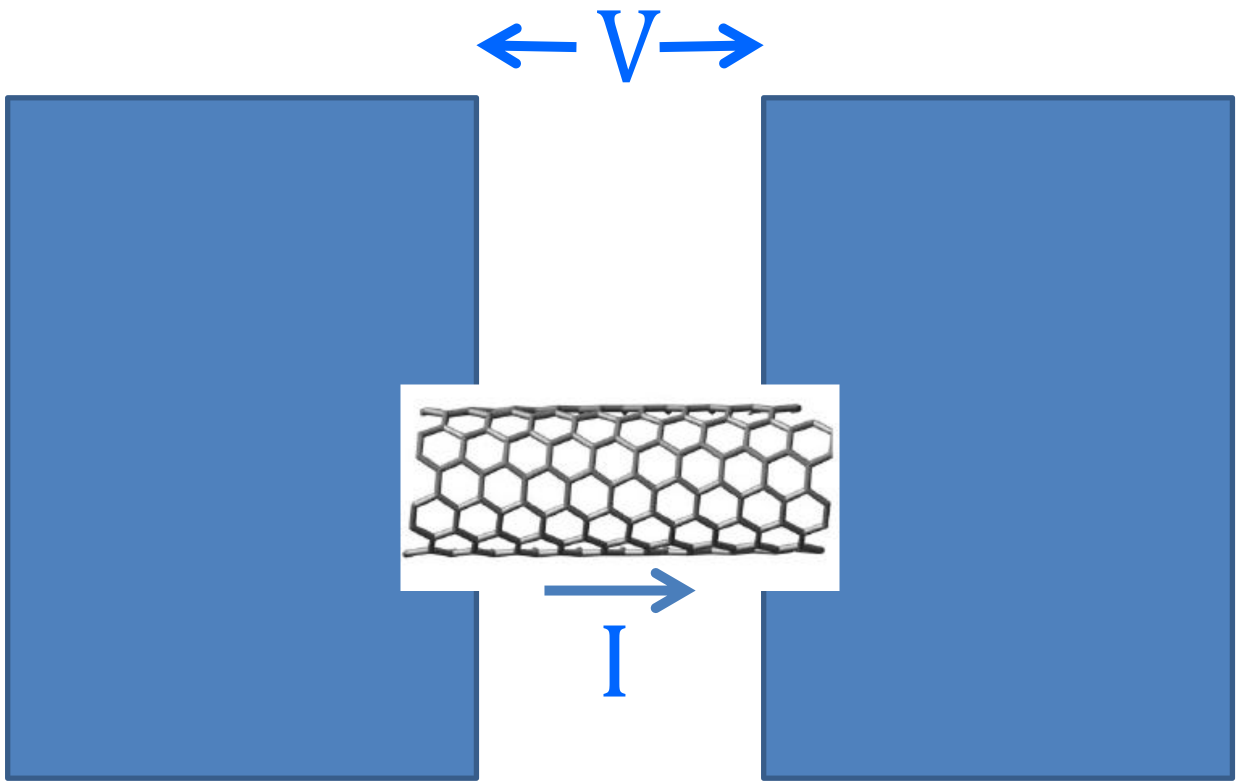
Bailey et al, PRL 100, 256802, 2008



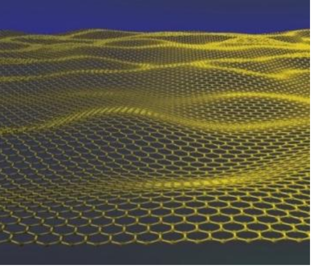
$$\vec{L} = \vec{r} \times \vec{p}$$

torque: $$\vec{\tau} = \frac{d\vec{L}}{dt} = \vec{r} \times \vec{F}$$

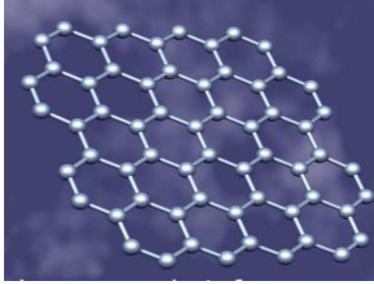
proposed device



(n,1) helical nanotube



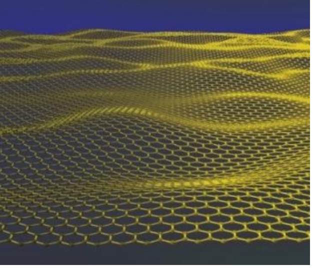
outline



1.helical nanotube (n,1)

2.energy spectrum

3. applied voltage *V*



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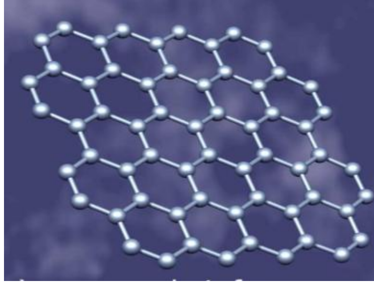

1. helical nanotube (n,1)

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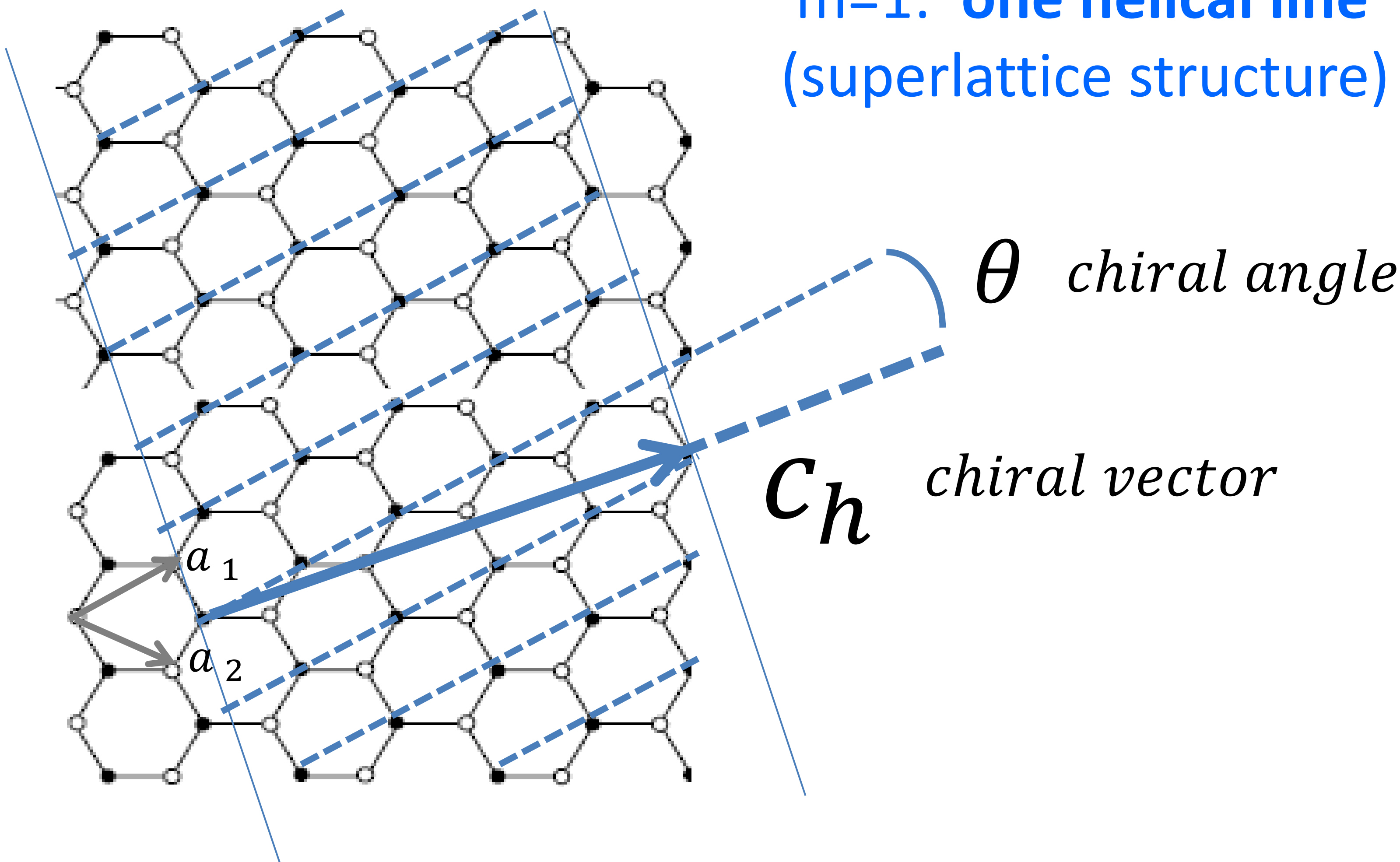
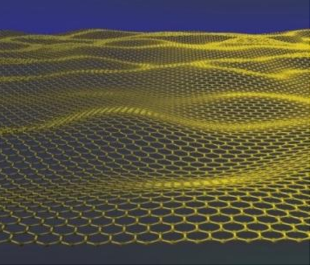
e.g. (4,1)


m=1: **one helical line**
(superlattice structure)
θ chiral angle
c_h chiral vector
a_1
a_2



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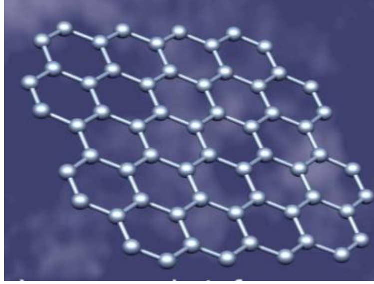

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(n,m) nanotube

$$k_s = k_\perp \cos\theta + k_\parallel \sin\theta$$

$$E(k_s) = \pm\gamma\sqrt{1 + 4\cos\frac{k_s a}{2}\cos\left(\frac{2n+m}{2m}k_s a - \frac{2\pi q}{m}\right) + 4\cos^2\frac{k_s a}{2}}\,, \quad k_\perp = \frac{2\pi q}{C_h}$$

Kibis et al, PRB 71, 035411, 2005

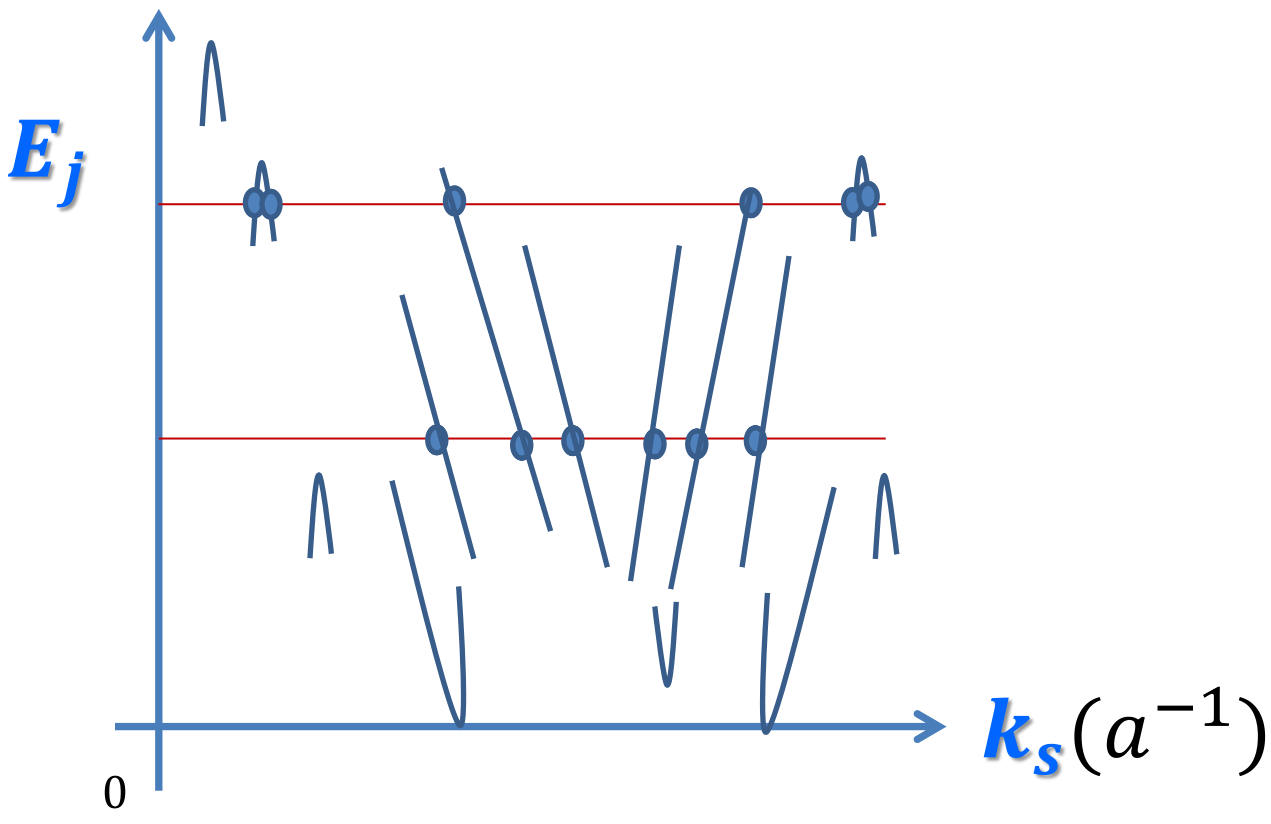
For the (n,1) chiral nanotube (m=1) the dispersion becomes independent of q

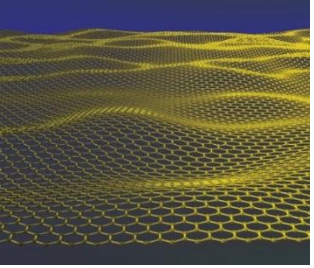
$$E_j(k_s) = (-1)^j\gamma\sqrt{1 + \cos\frac{(n+1)k_s a}{2}\cos\frac{n\,k_s a}{2}\cos\frac{k_s a}{2}}\,,$$

j=1 valence band and j=2 conduction band

for (n,1) energy E_j vs. k_s

$$E_j(k_s) = (-1)^j \gamma \sqrt{1 + \cos\frac{(n+1)k_s a}{2} \cos\frac{n\, k_s a}{2} \cos\frac{k_s a}{2}}, \quad j = 1,2$$





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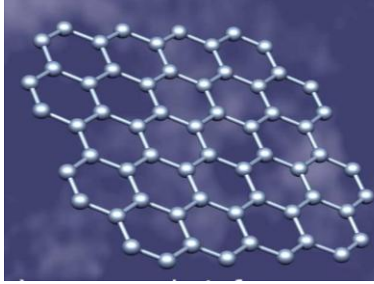


1. helical nanotube (n,1)

2. energy spectrum

3. applied voltage V

current

$$I = \frac{e}{h} \int dE \sum_i s_i f_{s_i}(E) \left(1 - f_{s_i}(E)\right)$$

i: channel index characterized by $k_{\perp,i}, k_{\parallel,i}$

E: electronic energy, $s_i = \mathrm{sgn}\left(v_{\parallel,i}\right)$, $v_{\parallel,i} = \frac{1}{\hbar} \frac{\partial E}{\partial k_{\parallel,i}}$

$f_{s_i}(E) = \frac{1}{1 + exp\frac{E - \mu - s_i V/2}{k_B \mathrm{T}}}$ Fermi-Dirac

μ: average chemical potential, *V*: bias potential

motion from lead to lead s_i to lead $-s_i$

force

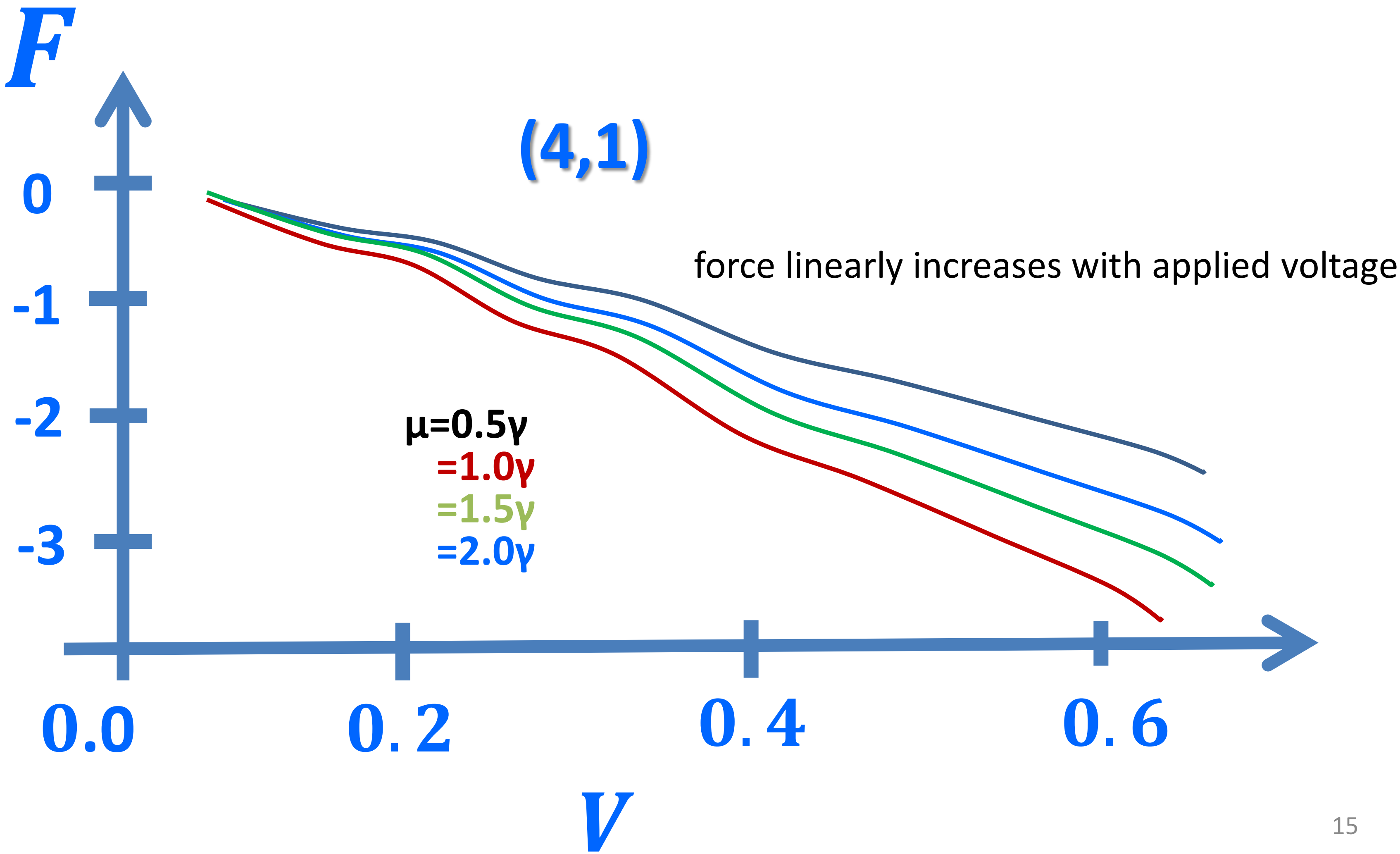
$$F = -\frac{1}{h}\int dE \sum_i m\, v_{\perp,i} f_{s_i}(E)\left(1 - f_{s_i}(E)\right)$$

each electron acquires momentum $mv_{\perp,i}r_0$,
$r_0$is the radius of nanotube

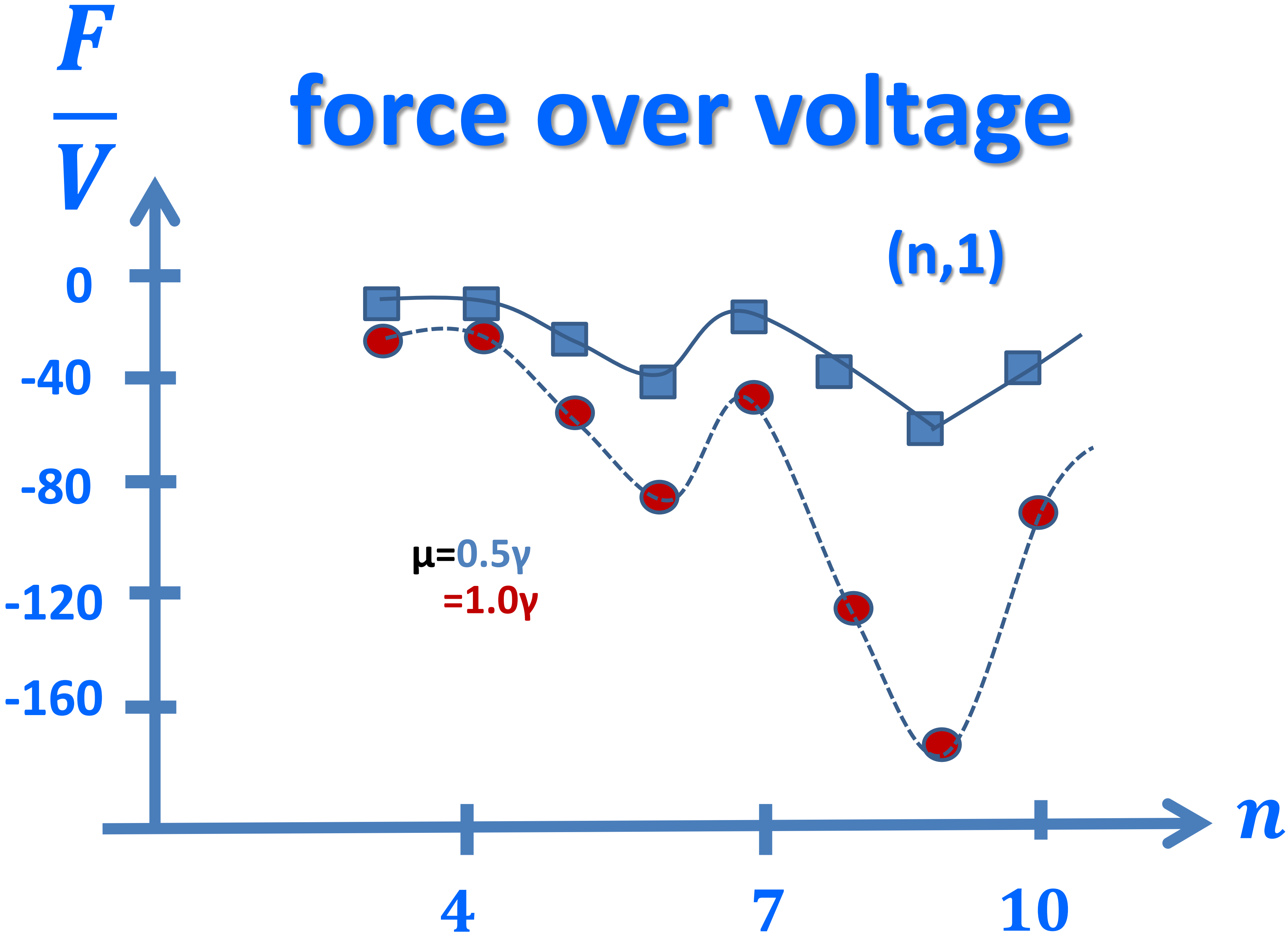
$$v_{\parallel,i} = \frac{1}{\hbar}\left(\frac{\partial E}{\partial k_s}\right)_i \sin\theta$$
$$v_{\perp,i} = \frac{1}{\hbar}\left(\frac{\partial E}{\partial k_s}\right)_i \cos\theta$$

correlation between longitudinal and transverse velocities

force vs. voltage



force over voltage



conclusions

- ✓ **ballistic transport** in chiral (n,1) nanotubes (helical) carbon nanotubes with no defects can lead to torque
- ✓ **torque** $\vec{\tau} = d\vec{L}/dt$ produced by the current **rotates** the nanotube around its axis if the force can overcome friction
- ✓ conditions to build such nanorotator **devices**