Mesoscopic Nano-Electro-Mechanics of Shuttle Systems

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- Lecture1: Mechanically assisted single-electronics
- Lecture2: Quantum coherent nano-electro-mechanics
- Lecture3: Mechanically assisted superconductivity

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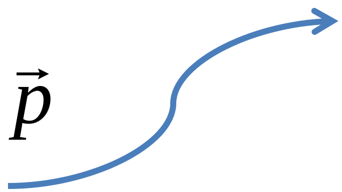
Lecture 2
Quantum Nano-Electromechanics

Outline

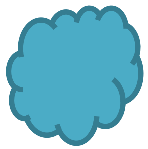
- *Quantum coherence of electrons*
- *Quantum coherence of mechanical displacements*
- *Mechanically induced quantum interferrence of electrons*

Quantum Coherence of Electrons

$\vec{r}, \vec{p}$



Classical approach



$$\delta p \delta x \geq \frac{\hbar}{2}$$

Heisenberg principle in quantum approach

Formalization of Heisenberg's principle:

$\{\hat{A}\}$ operators for physical variables

$\{\psi_\alpha\}$ eigenfunctions – quantum states

$\psi_{\vec{p}}(\vec{r}) = Ce^{i\frac{\vec{p}\vec{r}}{\hbar}}$ quantum state with definite momentum

$\chi(\vec{r}) = \sum_{\vec{p}} a_{\vec{p}} \psi_{\vec{p}}(\vec{r})$ In this state the momentum experiences quantum fluctuations

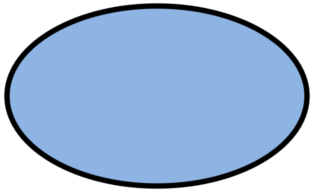
Stationary Quantum States

Hamiltonian of a single electron: $$\hat{H} = \frac{\hat{p}^2}{2m} + U(\vec{r}); \quad \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial \vec{r}}$$

Stationary quantum states: $$\hat{H}\psi_\alpha = E_\alpha \psi_\alpha$$

Second Quantization

- Spatial quantization ⇔ discrete quantum numbers



- Due to quantum tunneling the number of electrons in the body experiences quantum fluctuations and is not an integer
- One therefore needs a description that treats the particle number **N** as a quantum variable

Wave function for system of **N** electrons: $\psi_{N\{\alpha_n\}}(\vec{r})$

Creation and annihilation operators

$$\hat{a}_\alpha{}^+\psi_N(\{\vec{r}_n\}) = \psi_{N+1}(\{\vec{r}_n\})$$
$$\hat{a}_\alpha\psi_N(\{\vec{r}_n\}) = \psi_{N-1}(\{\vec{r}_n\})$$

$$\hat{N} = \sum_{\{\alpha\}} \hat{n}_\alpha \equiv \sum_{\{\alpha\}} a_\alpha^+ a_\alpha$$
$$\hat{H} = \sum_\alpha \hat{n}_\alpha \varepsilon_\alpha$$

$$\left[a_\alpha^+, a_\beta\right]_+ = \delta_{\alpha,\beta} \quad \text{fermions}$$
$$\left[a_\alpha^+, a_\beta\right]_- = \delta_{\alpha,\beta} \quad \text{bosons}$$

Field Operators

$$\hat{\psi}^+(\vec{r}) = \sum_\alpha a_\alpha^+ \varphi_\alpha(\vec{r}); \quad \hat{n}(\vec{r}) = \hat{\psi}^+(\vec{r})\hat{\psi}(\vec{r})$$

$$\hat{H} = \int d\vec{r}\, \hat{\psi}^+(\vec{r}) \hat{H}(r) \hat{\psi}(\vec{r})$$

$$\left[\hat{\psi}(\vec{r}_1), \hat{\psi}^+(\vec{r}_2)\right]_+ = \delta(\vec{r}_1 - \vec{r}_2)$$

Density Matrix

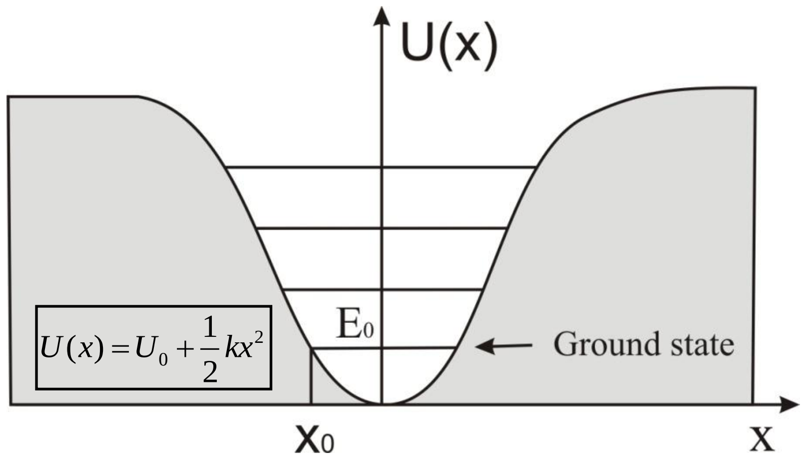
$$A = Sp\{\hat{\rho}\hat{A}\}; \qquad i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}]$$

Louville – von Neumann equation

Zero-Point Oscillations

Consider a classical particle which oscillates in a quadratic potential well. Its equilibrium position, **X=0**, corresponds to the potential minimum **E=min{U(x)}**.

A quantum particle can not be localized in space. Some "residual oscillations" are left even in the ground states. Such oscillations are called zero point oscillations.



Amplitude of zero-point oscillations:

$$x_0 = \sqrt{\hbar / m\omega}$$

Classical motion:

$$m\frac{d^2x}{dt^2} = -\frac{\partial U}{\partial x} \equiv -kx \qquad \omega = \sqrt{\frac{k}{m}}$$

Quantum motion:

$$p \sim \hbar / x \Rightarrow E(x) = \hbar^2 / 2mx^2 + kx^2 / 2$$

$$E(x_0) = \min\{E(x)\}$$

Classical vs quantum description: the choice is determined by the parameter x_0 / d

where **d** is a typical length scale for the problem. "Quantum" when $x_0 / d \sim 1$

Quantum Nanoelectromechanics of Shuttle Systems

$$\delta x \delta p \cong \hbar \qquad \delta x \cong 2x_0 \equiv \sqrt{\frac{2\hbar}{M\omega}}$$

If $\left| R(x+\delta x) - R(x) \right| >> R(x)$ then quantum fluctuations of the grain significantly affect nanoelectromechanics.

Conditions for Quantum Shuttling

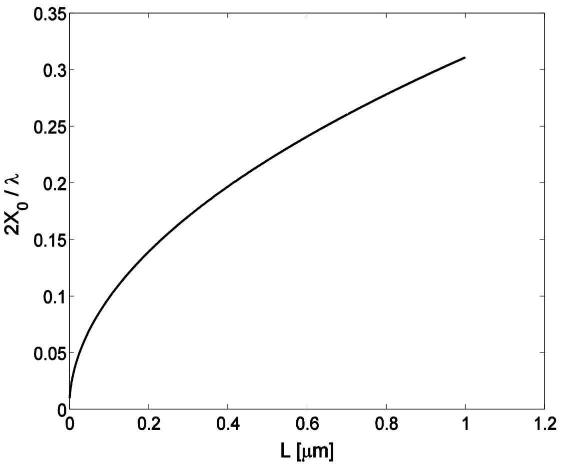
$$x_0 = \sqrt{\frac{\hbar}{2M\omega}} \qquad \frac{2x_0}{\lambda} \tilde{>} 1$$

λ – Tunneling length

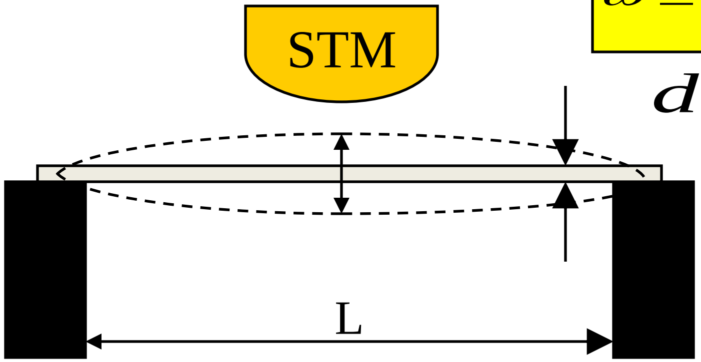
1. Fullerene based SET

$$\frac{x_0}{\lambda} \cong 0.1$$ → Quasiclassical shuttle vibrations.

$\omega \cong 1\,\mathrm{THz}$



2. Suspended CNT



$$\omega \cong 10^{14}\ \mathrm{Hz} \left(\frac{d}{L}\right)^2$$

$d \cong 1\,\mathrm{nm}$

$\omega \cong 10^8$ - 10^9 Hz for SWNT with $L \cong 1\mu m$

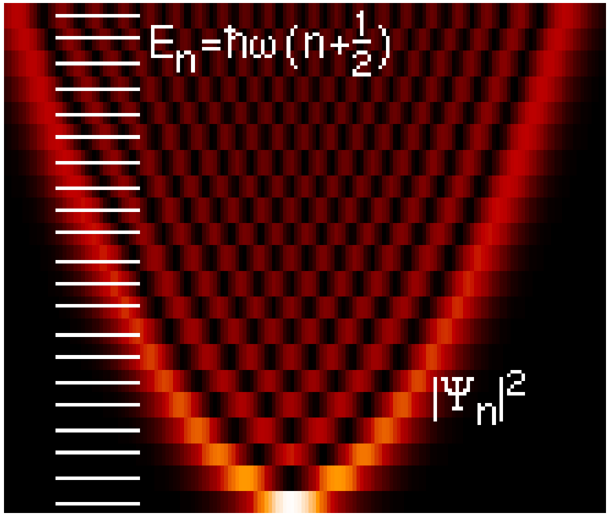
Quantum Harmonic Oscillator

$$H = \frac{\hat{p}^2}{2M} + \frac{1}{2} M\omega^2 \hat{x}^2$$

$$\hat{p} = -i\hbar \frac{d}{dx}$$

$$|n> = \left(\frac{1}{2^n n!}\right)^{\frac{1}{2}} \left(\frac{M\omega}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left(-\frac{M\omega x^2}{2\hbar}\right) H_n\left(x\sqrt{\frac{M\omega}{\hbar}}\right)$$

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$



Probability densities $|\psi_n(x)|^2$ for the boundeigenstates, beginning with the ground state (***n* = 0**) at the bottom and increasing in energy toward the top. The horizontal axis shows the position ***x***,and brighter colors represent higher probability densities.

Ledder operators

$$a = \sqrt{\frac{M\omega}{2\hbar}}\left(\hat{x} + \frac{i}{M\omega}\hat{p}\right)$$

$$a^+ = \sqrt{\frac{M\omega}{2\hbar}}\left(\hat{x} - \frac{i}{M\omega}\hat{p}\right)$$

$$a|n> = \sqrt{n}\,|n-1>$$

$$a^+|n> = \sqrt{n+1}\,|n+1>$$

$$\hat{x} = \sqrt{\frac{\hbar}{2M\omega}}\left(a + a^+\right)$$

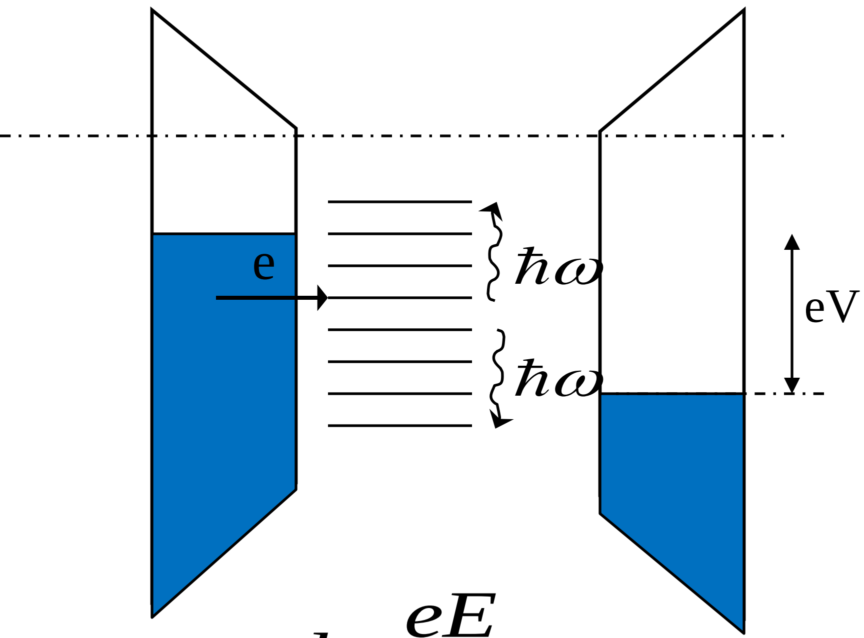
$$\hat{p} = i\sqrt{\frac{\hbar}{2M\omega}}\left(a^+ - a\right)$$

$$H = \hbar\omega\left(a^+ a + 1/2\right)$$

$$[a, a^+] = 1$$

Eigenstate of oscillator is a ideal gas of elementary excitations – vibrons, which are a bose particles.

Quantum Shuttle Instability

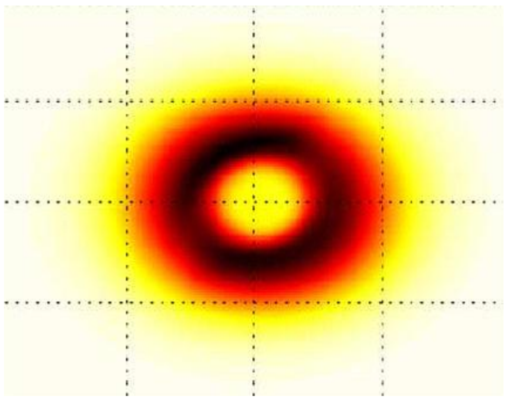


$$d = \frac{eE}{2k}$$

Shift in oscillator position caused by charging it by a single electron charge.

Quantum vibrations, generated by tunneling electrons, remain undamped and accumulate in a **coherent "condensate"** of phonons, which is classical shuttle oscillations.

$$\gamma < \gamma_{\text{thr}} \equiv \Gamma \frac{d}{\lambda}$$



Phase space trajectory of shuttling. From **Ref. (3)**

References:

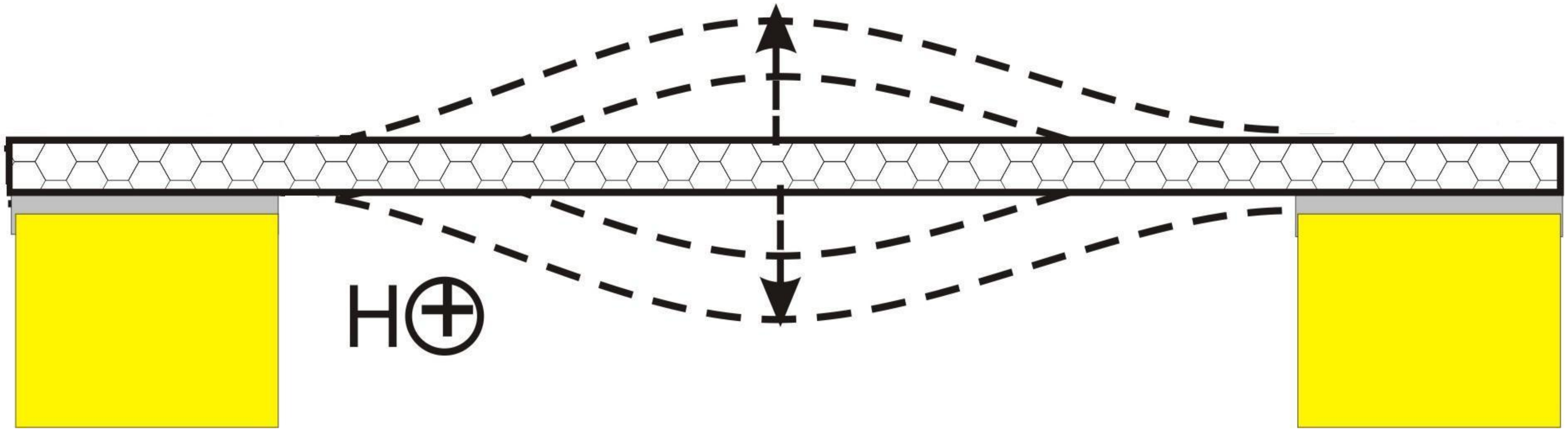
(1) D. Fedorets *et al.* Phys. Rev. Lett. 92, 166801 (2004)

(2) D. Fedorets, Phys. Rev. B **68**, 033106 (2003)

(3) T. Novotny *et al.* Phys. Rev. Lett. **90** 256801 (2003)

How to Detect Nanomechanical Vibrations in the Quantum Limit?

Try new principles for sensing the quantum displacements!

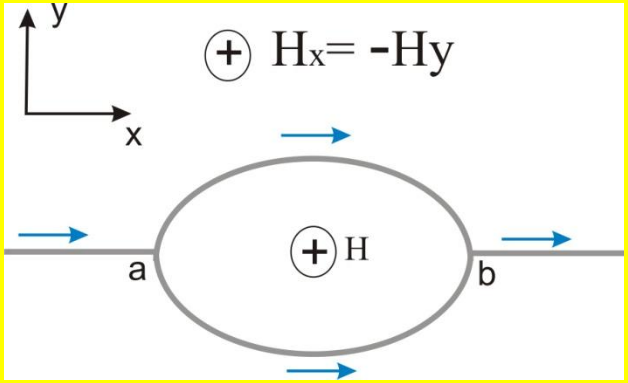


Consider the transport of electrons through a suspended, vibrating carbon nanotube beam in a transverse magnetic field **H**. What will the effect of **H** be on the conductance?

Shekhter R.I. et al. PRL **97**(15): Art.No.156801 (2006).

Aharonov-Bohm Effect

The particle wave, incidenting the device from the left splits at the left end of the device. In accordance with the superposition principle the wave function at the right end will be given by:



$$\psi(b) = \sum_i \psi_i(b) = \psi_{\vec{A}=0}(b) \sum_i \exp\{i\alpha_i\}$$

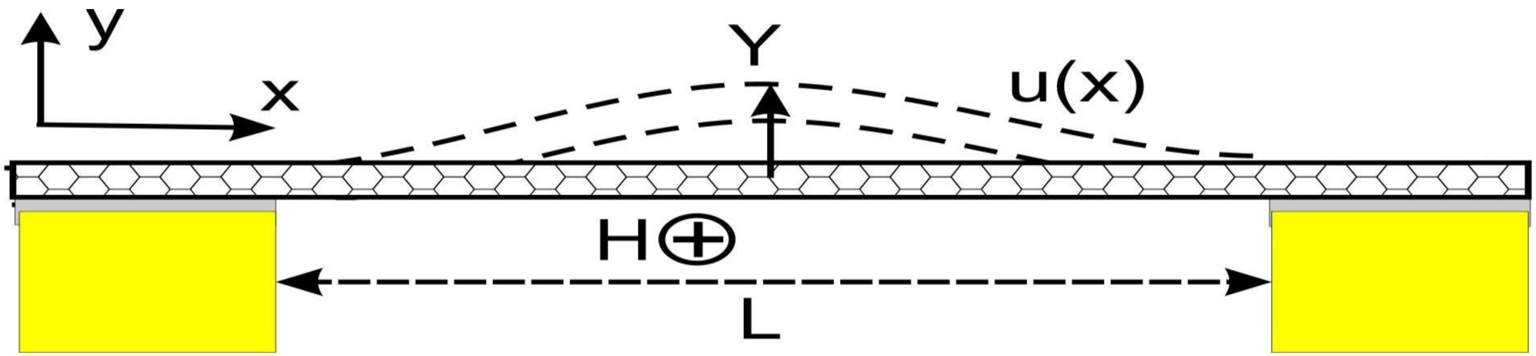
$$\alpha_i(x) = \frac{e\hbar}{c}\int_{L_i} d\vec{l}\,\vec{A}$$

$$\alpha_2 - \alpha_1 = 2\pi\frac{\Phi}{\Phi_0}; \quad \Phi = \frac{1}{2\pi}\oint_L d\,\vec{l}\cdot\vec{A} \equiv \oiint_S d\vec{s}\;\vec{H}; \quad \Phi_0 = \frac{2\pi c}{e\hbar} \Leftrightarrow \text{(flux quantum)}$$

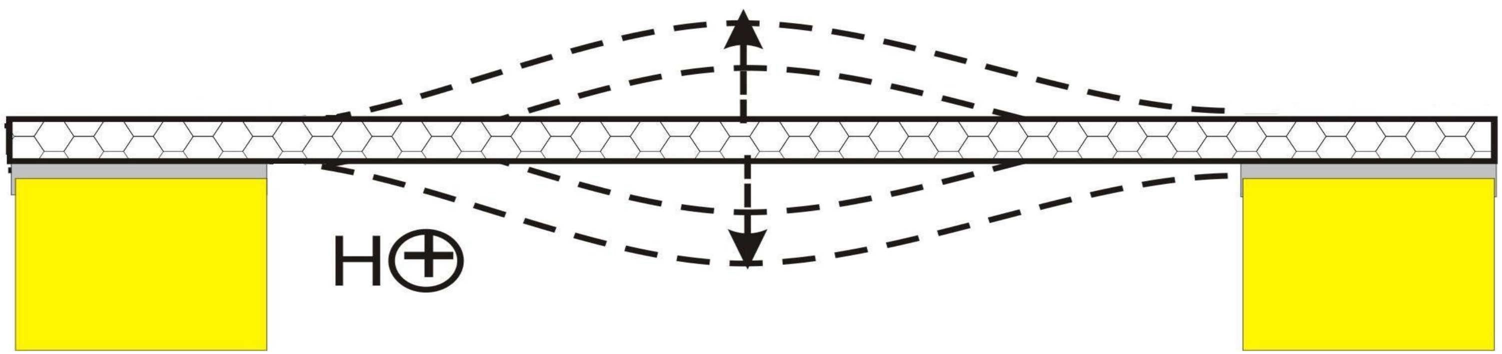
The probability for the particle transition through the device is given by:

$$|T|^2 = |\psi_{\vec{A}=0}|^2 \left\{\left(1+\cos\left(2\pi\frac{\Phi}{\Phi_0}\right)\right)^2 + \sin^2\left(2\pi\frac{\Phi}{\Phi_0}\right)\right\}$$

Classical and Quantum Vibrations



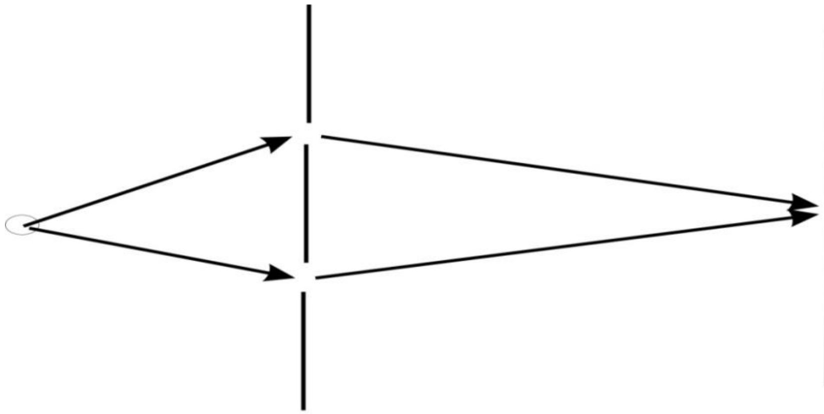
In the classical regime the **SWNT** fluctuations **u(x,t)** follow well defined trajectories.



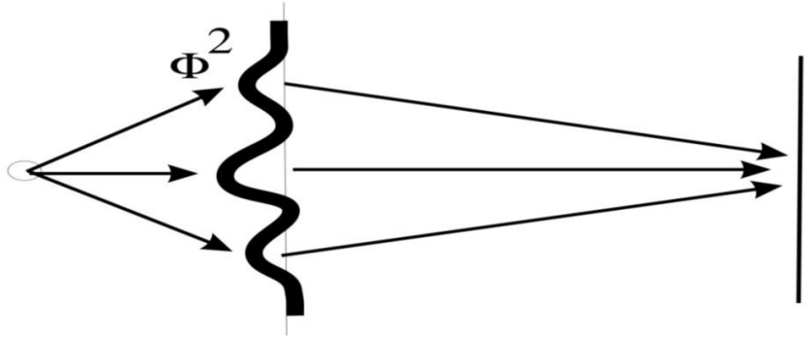
In the quantum regime the **SWNT** zero-point fluctuations (not drawn to scale) smear out the position of the tube.

Quantum Nanomechanical Interferometer

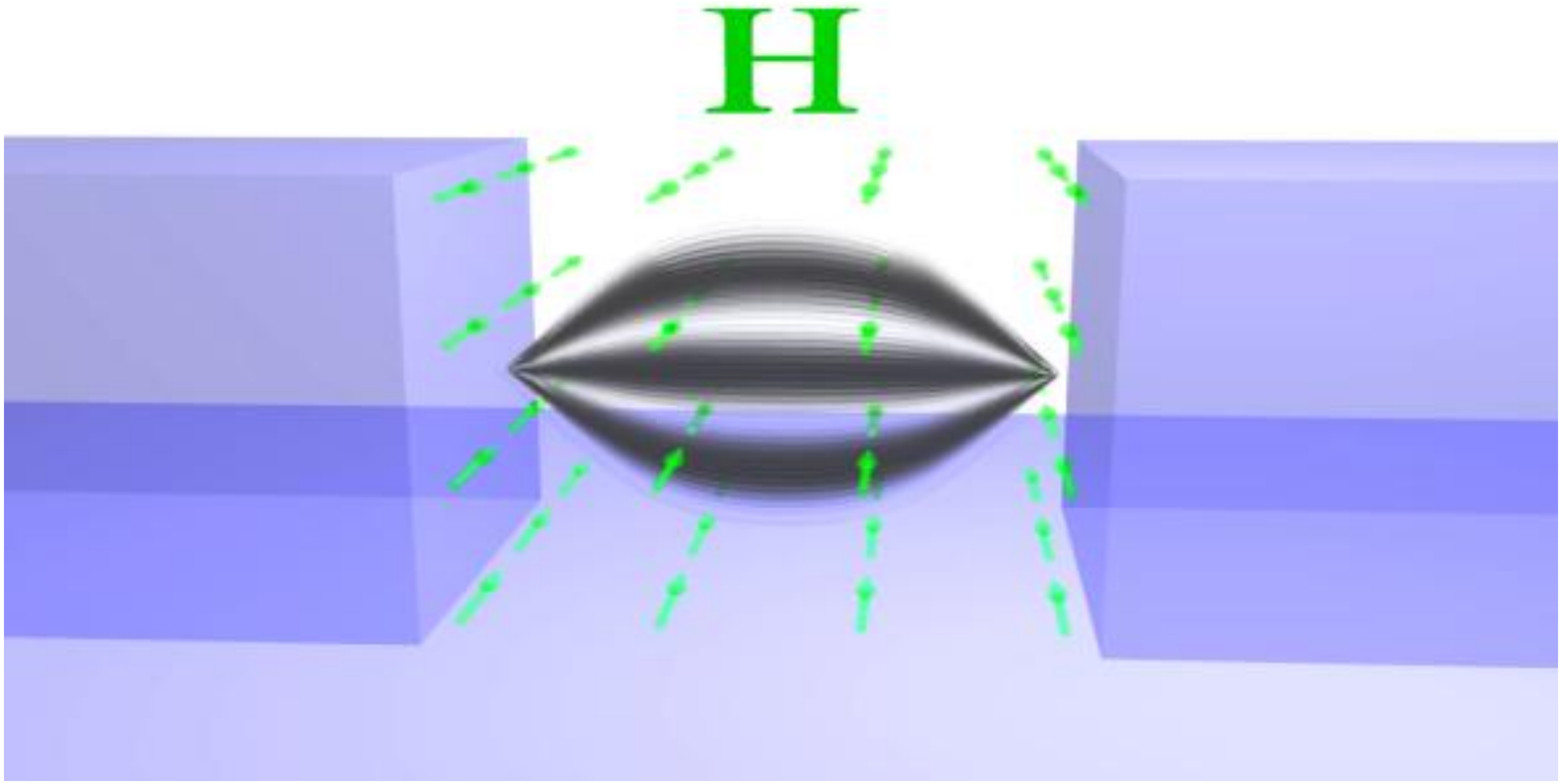
Classical interferometer



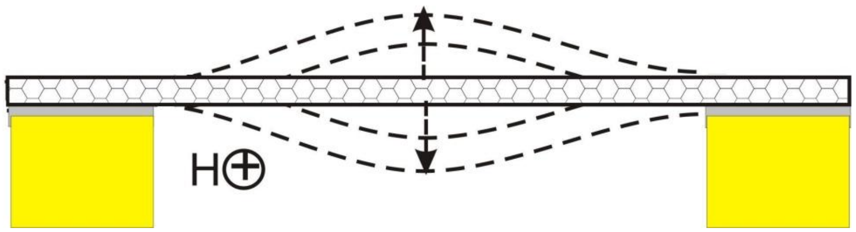
Quantum nanomechanical interferometer



Electronic Propagation Through Swinging Polaronic States



Coupling to the Fundamental Bending Mode

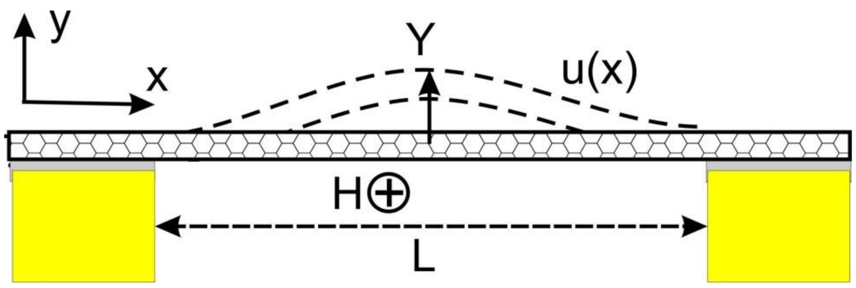


Only one vibration mode is taken into account

$$\hat{u}(x) = x_0 u_0(x)(\hat{b}^+ + \hat{b})/\sqrt{2} \; ; \quad x_0 = \left(\hbar^2 L^2 / \beta_0 \rho E I \right)^{1/4}$$

CNT is considered as a complex scatterer for electrons tunneling from one metallic lead to the other.

Tunneling through Virtual Electronic States on CNT



- Strong longitudinal quantization of electrons on CNT
- No resonance tunneling though the quantized levels *(only virtual localization of electrons on CNT is possible)*

Effective Hamiltonian

$$H = \sum_{\alpha,\sigma} \varepsilon_\alpha a^+_{\alpha,\sigma} a_{\alpha,\sigma} + \frac{\hbar\omega}{2}\hat{b}^+\hat{b} + (T_{eff} e^{i\Phi(\hat{b}^+ + \hat{b})} \sum_{\alpha,\alpha'} a^+_{\alpha,R} a_{\alpha',L} + h.c)$$

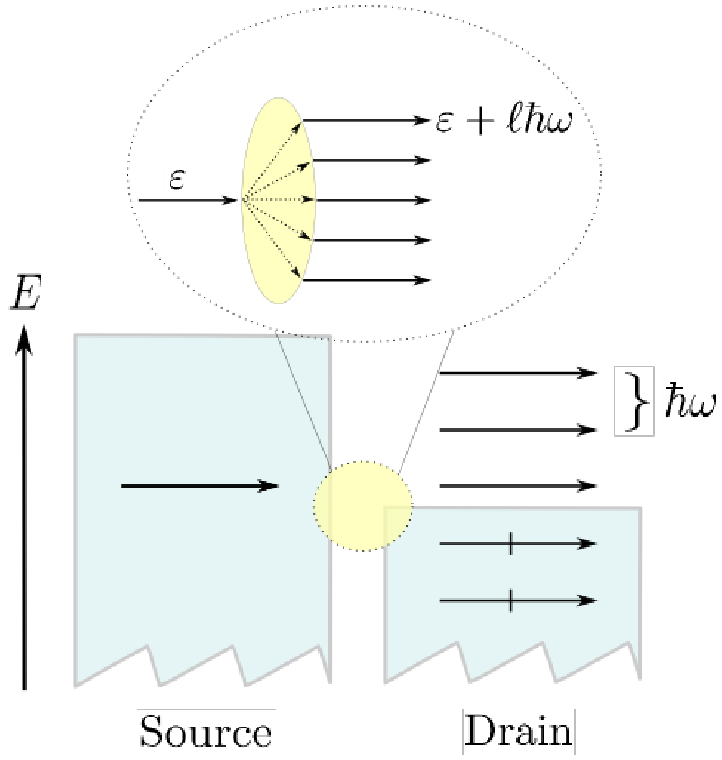
$$\Phi = gHLY_0 / \sqrt{2}\Phi_0 \qquad Y_0 = \sqrt{\hbar/2M\omega_0} \propto \sqrt{L} \qquad T_{eff} = \frac{T_L T_R^*}{E-\mu}$$

Calculation of the Electrical Current

$$I = G_0 \sum_{n=0}^{\infty} \sum_{l=-n}^{\infty} P(n) \,|\langle n | e^{i\Phi(\hat{b}^+ + \hat{b})} | n+l \rangle|^2 \times$$
$$\int d\varepsilon \left[f_l(\varepsilon)\left(1 - f_r(\varepsilon - l\hbar\omega)\right) - f_r(\varepsilon)\left(1 - f_l(\varepsilon - l\hbar\omega)\right)\right]$$

$$G/G_0 = \sum_{n=0}^{\infty} P(n) \,|\langle n | e^{i\Phi(\hat{b}^+ + \hat{b})} | n \rangle|^2 +$$
$$\sum_{n=0}^{\infty} \sum_{l=1}^{\infty} P(n) \,|\langle n | e^{i\Phi(\hat{b}^+ + \hat{b})} | n+l \rangle|^2 \frac{2l\hbar\omega / kT}{\exp(l\hbar\omega / kT) - 1}$$

Vibron-Assisted Tunneling through Suspended Nanowire



- Tunneling through vibrating nanowire is performed in both elastic and inelastic channels.
- Due to Pauli-principle, some of the inelastic channels are excluded.
- Resonant tunneling at small energies of electrons is reduced.
- Current reduction becomes independent of both temperature and bias voltage.

Linear Conductance

Vibrational system is in equilibrium

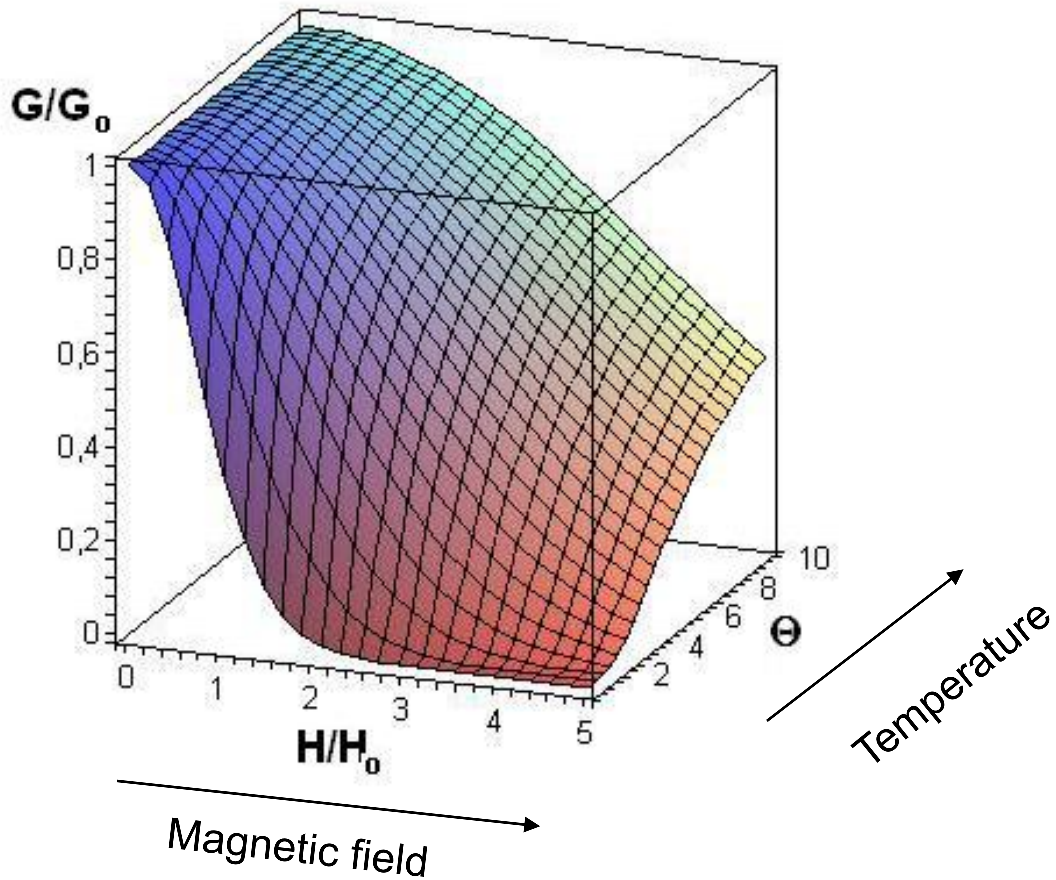
$$\frac{G}{G_0} \approx \exp\left\{-\left(\frac{\Phi}{\Phi_0}\right)^2\right\}, \quad \frac{\hbar\omega}{kT} >> 1$$

$$\frac{G}{G_0} \approx 1 - \frac{1}{6}\left(\frac{\Phi}{\Phi_0}\right)^2 \frac{\hbar\omega}{kT}, \quad \frac{\hbar\omega}{kT} << 1$$

$$\Phi = 4\pi g L x_0 H, \qquad \Phi_0 = h/e$$

For a **1 μm** long **SWNT** at ***T* = 30 mK** and ***H* ≈ 20 - 40 T** a relative conductance change is of about **1-3%**, which corresponds to a magneto-current of **0.1-0.3 pA**.

Quantum Nanomechanical Magnetoresistor

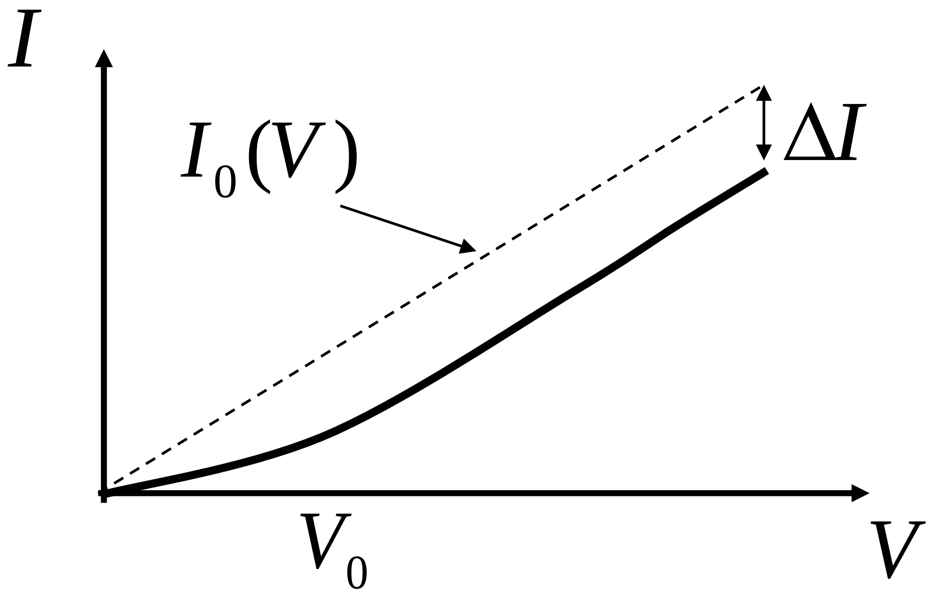


R.I. Shekhter et al., PRL **97**, 156801 (2006)

Magnetic Field Dependent Offset Current

$$I = I_0(V) - \Delta I;$$

$$\frac{\Delta I}{I_0} \approx \frac{\hbar\omega}{eV}\left(\frac{\Phi}{\Phi_0}\right)^2$$



$$eV >> \hbar\omega\left(\frac{\Phi}{\Phi_0}\right)^2$$

$$eV_0 = \hbar\omega\left(\frac{\Phi}{\Phi_0}\right)^2$$

Model

$$H = \sum_{\sigma=L,R} H_\sigma + H_e + H_m + \sum_{\sigma=L,R} T_\sigma$$

$$H_\sigma = \sum_\alpha \varepsilon_\alpha a^+_{\alpha,\sigma} a_{\alpha,\sigma}$$

$$H_e = \int d^3 r \left\{ -\frac{\hbar^2}{2m} \psi^+(r) \left(\frac{\partial}{\partial r} - \frac{ie}{c\hbar} A \right)^2 \psi(r) + U\big(y - u(x,z)\big) \psi^+(r) \psi(r) \right\}$$

$$\psi^+(\vec{r}) = \sum_q a_q^+ \varphi_q(\vec{r})$$

$$H_m = \int_{-L/2}^{L/2} dx \left\{ \frac{1}{2\rho} \hat{\pi}^2 + \frac{EI}{2} \left(\frac{\partial^2 u(x)}{\partial x^2} \right)^2 \right\}$$

$$\hat{\pi} = -i\hbar \frac{d}{du}$$