COLLEGE ON

PHYSICS OF NANO-DEVICES

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*Quantum Nanoelectromechanics Due to
Tunneling of a Single Electron*

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Mechanically Assisted Single-Electronics

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Lecture 2

Quantum Nanoelectromechanics
due toTunneling of Single Electrons

Outline

- *Conditions for Quantum Shuttling*

- *Formulation of the problem*

- *Quantum kinetic equation*

- *Shuttle instability in the quantum limit*

- *Semiclassical and quantum shuttle vibrations*

- *Interferometry of quantum nanovibrations*

The Electronic Shuttle
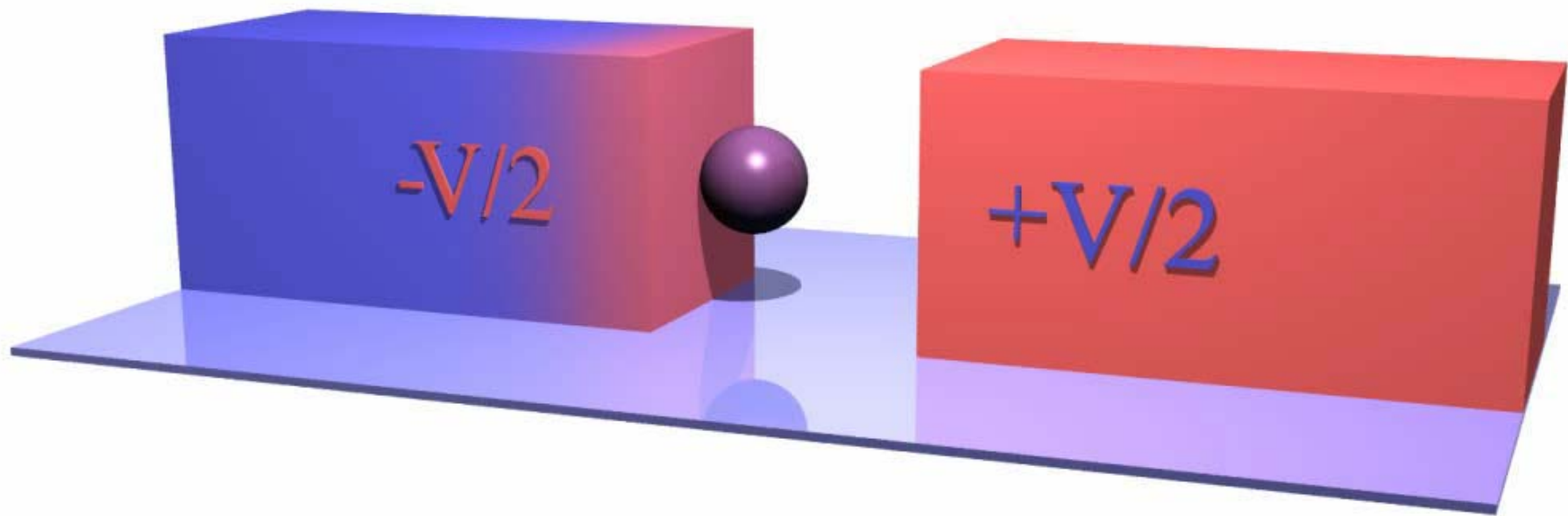
Conditions for Quantum Shuttling

Quantum Nanoelectromechanics of Shuttle Systems

$$\delta X \delta P \cong \hbar$$

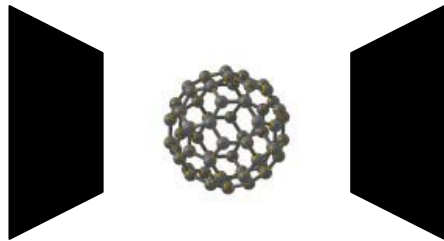$$\delta X \cong 2 X_0 \equiv \sqrt{\frac{2\hbar}{M\omega}}$$

If $\dfrac{R(X + \delta X)}{R(X)} \gg 1$ then quantum fluctuations of the grain significantly affect nanoelectromechanics.

Conditions for Quantum Shuttling

$$\frac{2X_0}{\lambda} \gtrsim 1$$

$$\lambda - \text{Tunneling length}$$

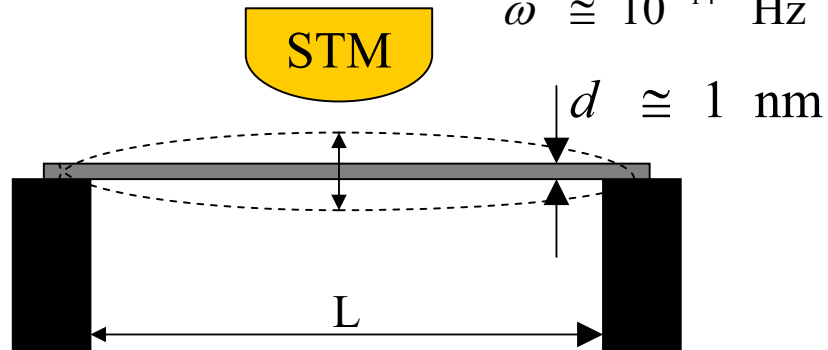## 1. Fullerene based SET

$$\omega \cong 1 \text{ THz}$$

$$\frac{X_0}{\lambda} \cong 0.1$$
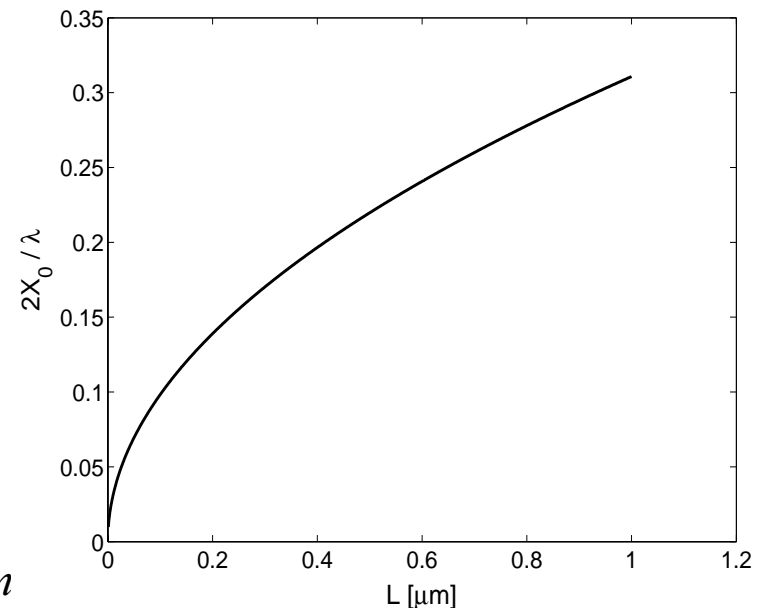
➡ Quasiclassical shuttle vibrations.
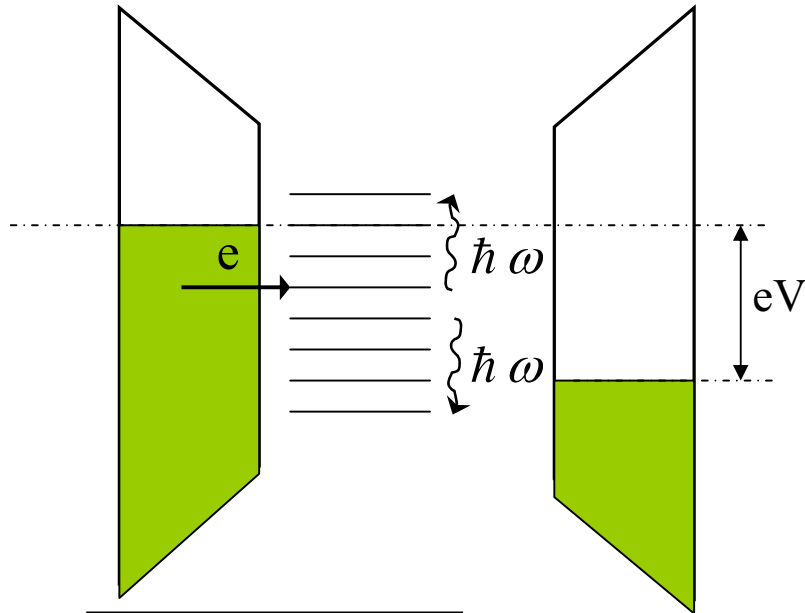
2. Suspended CNT

STM

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

$$d \cong 1 \text{ nm}$$

L

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

Quantum Shuttle Instability

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

Phase space trajectory of shuttling. From Ref. (3)
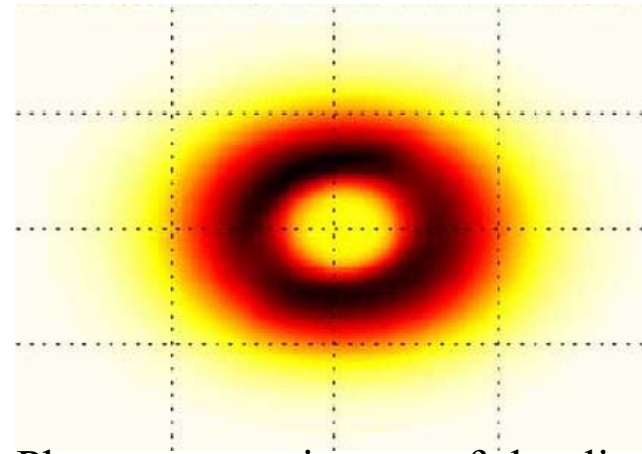
$$\gamma < \gamma_{thr} \equiv \Gamma \frac{d}{\lambda}$$

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

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

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)

Theory of Quantum Shuttle

The Hamiltonian:

$$H = H_{Leads} + H_{Dot} + H_T$$

$$H_{Leads} = \sum_{\alpha,k} (\varepsilon_{\alpha k} - \mu_\alpha) a_{\alpha k}^+ a_{\alpha k}$$

$$H_{Dot} = [\varepsilon_0 - eE\hat{x}] c^+ c + H_v,$$

$$H_T = \sum_{\alpha,k} T_\alpha(\hat{x})(a_{\alpha k}^+ c + c^+ a_{\alpha k})$$

$$H_v = [\hat{p}^2 + \hat{x}^2]/2$$
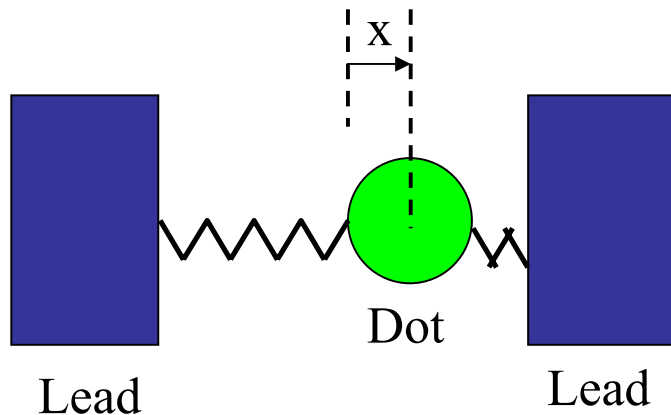
$$T_{L,R}(x) = T_0 e^{\mp x/\lambda}, \quad \mu_{L,R} = \mu \pm eV/2$$

Time evolution in
Schrödinger picture:

$$\partial_t \hat{\sigma}(t) = -i[H, \hat{\sigma}(t)]$$

Total density operator

Reduced density operator

$$\hat{\rho}(t) \equiv Tr_{leads} \hat{\sigma}(t) \equiv \begin{pmatrix} \hat{\rho}_0(t) & \hat{\rho}_{01}(t) \\ \hat{\rho}_{10}(t) & \hat{\rho}_1(t) \end{pmatrix}$$

Generelized Master Equation

$\hat{\rho}_0:$ density matrix operator of the *uncharged* shuttle

$\hat{\rho}_1:$ density matrix operator of the *charged* shuttle

At large voltages the equations for $\hat{\rho}_0, \hat{\rho}_1$ are local in time:

$$\partial_t \hat{\rho}_0 = -i[H_v + eE\hat{x}, \hat{\rho}_0]_- - \{\Gamma_L(\hat{x}), \hat{\rho}_0\}_+ + \sqrt{\Gamma_R(\hat{x})}\hat{\rho}_1\sqrt{\Gamma_R(\hat{x})} + L_\gamma\hat{\rho}_0$$

Free oscillator dynamics   Electron tunnelling   Dissipation

$$\partial_t \hat{\rho}_1 = -i[H_v - eE\hat{x}, \hat{\rho}_1]_- - \{\Gamma_R(\hat{x}), \hat{\rho}_1\}_+ + \sqrt{\Gamma_L(\hat{x})}\rho_0\sqrt{\Gamma_L(\hat{x})} + L_\gamma\hat{\rho}_1$$

$$L_\gamma\hat{\rho}_\alpha \equiv \frac{i\gamma}{2}[\hat{x}, \{\hat{p}, \hat{\rho}_\alpha\}] - \frac{\gamma}{2}[\hat{x}, [\hat{x}, \hat{\rho}_\alpha]]$$

$\hat{\rho}_- \equiv \hat{\rho}_0 - \hat{\rho}_1:$ describes shuttling of electrons

$\hat{\rho}_+ \equiv \hat{\rho}_0 + \hat{\rho}_1:$ describes vibrational space.

Approximation: $x_0/\lambda \ll 1, \quad eE/k\lambda \ll 1, \quad \gamma \ll 1$

Shuttle Instability

After linearisation in x (using the small parameter x_0/λ) one finds:

$$\dot{x} = p$$

$$\dot{p} = -x - \gamma p - \frac{d}{2x_0} n_-$$

$$\dot{n}_- = -\frac{\Gamma}{\hbar} n_- + \frac{2\Gamma x_0}{\hbar \lambda} x$$

$$x(t) \equiv x_0^{-1} Tr\left[\hat{\rho}_+(t)\hat{x}\right]$$

$$p(t) \equiv \frac{x_0}{\hbar} Tr\left[\hat{\rho}_+(t)\hat{p}\right]$$

$$n_-(t) = 1 - Tr\left[\hat{\rho}_1(t)\right]$$

<u>Result</u>: *an initial deviation from the equilibrium position grows exponentially if the dissipation is small enough*:

$$x(t) \propto \exp(\alpha t);$$

$$\alpha = (\gamma_{thr} - \gamma)/2; \quad \gamma < \gamma_{thr} \equiv \frac{\Gamma}{\hbar} \frac{d}{\lambda}$$

Semiclassical and Quantum Regimes of Shuttling

Pumping of the energy

$$W_{cl}(E) \approx \frac{eE\lambda\Gamma(x)}{\hbar},$$

$$\delta x_q \approx \hbar \Big/ \sqrt{2m\omega}$$

$\delta\Gamma_q \approx$ Quantum correction to the pumping results
in quantum part of the shuttling energy δW_q

$$\delta W_q = \frac{E_c}{E} W_{cl}$$

$$\delta W_q = W_{cl}(E_c)$$

$$E_c \equiv \Gamma\hbar / eM\omega\lambda^3 \propto \hbar$$

1). $E \gg E_c$ − Semiclassical limit

1). $E \leq E_c$ − Quantum limit

Stationary Shuttle Vibrations

Electronic pumping of the vibrational energy drives oscillator to a excited states with a large energy.

Questuion: Does such pumping restore a classical shuttle vibrations?

Wigner Function Representation

$$W_\pm(x,p) \equiv \frac{1}{2\pi} \int\limits_{-\infty}^{+\infty} d\xi\, e^{-ip\xi} \langle x + \frac{\xi}{2} | \hat{\rho}_\pm | x - \frac{\xi}{2} \rangle$$

$|x\rangle$ — *Eigenfunction of the operator of coordinate*

Kinetic Equation in Wigner Representation
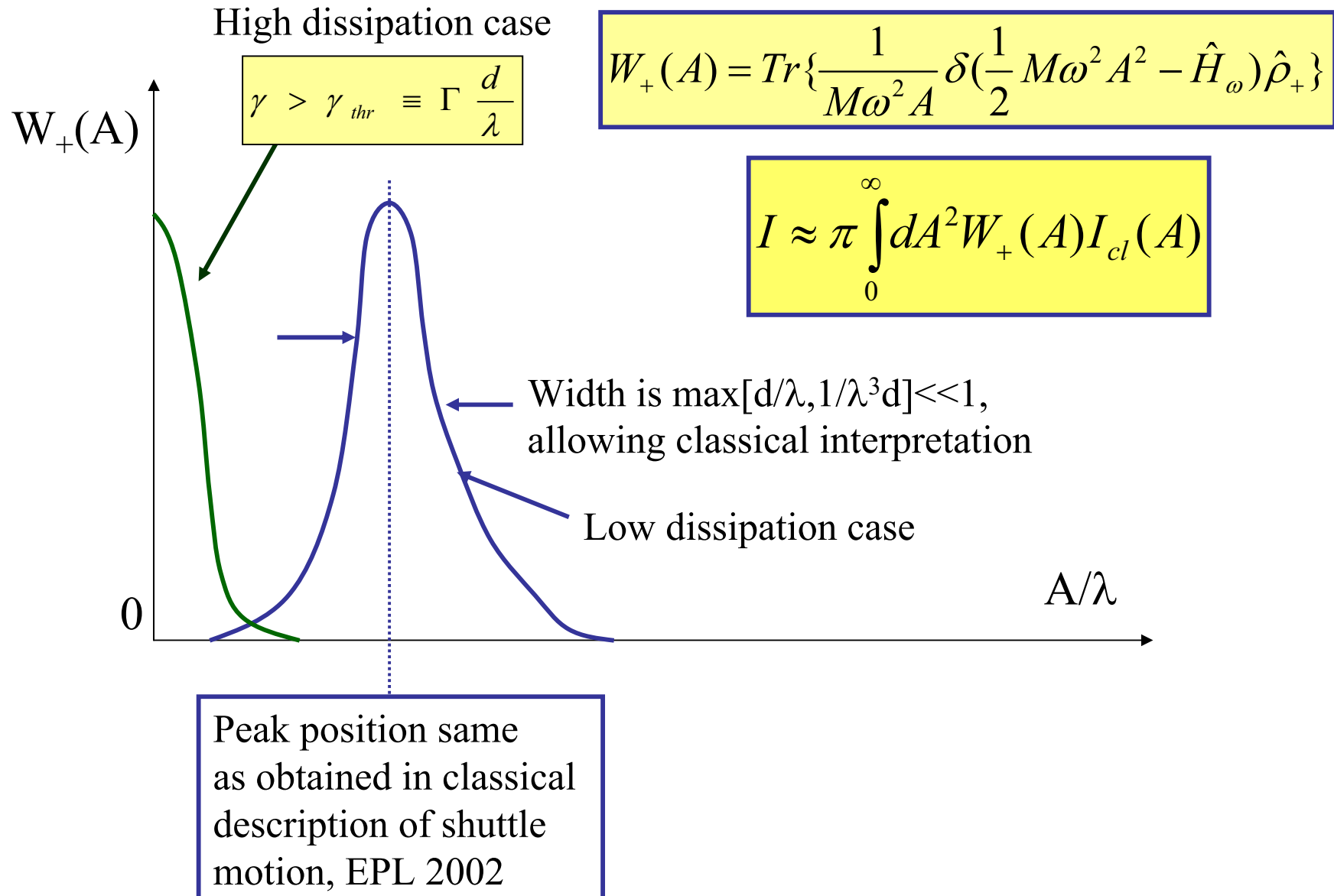
Performing the Wigner transformation of the quantum kinetic equation for the density matrix one gets the equation for the Wigner functions

$$\dot{W}_+ = \left(X\partial_P - P\partial_X + \hat{L}_1 \right) W_+ + \hat{L}_2 W_-$$

$$\dot{W}_- = \left(X\partial_P - P\partial_X + \hat{L}_1 - \Gamma_+(X) \right) W_- + \left(\hat{L}_2 + \Gamma_-(X) \right) W_+$$
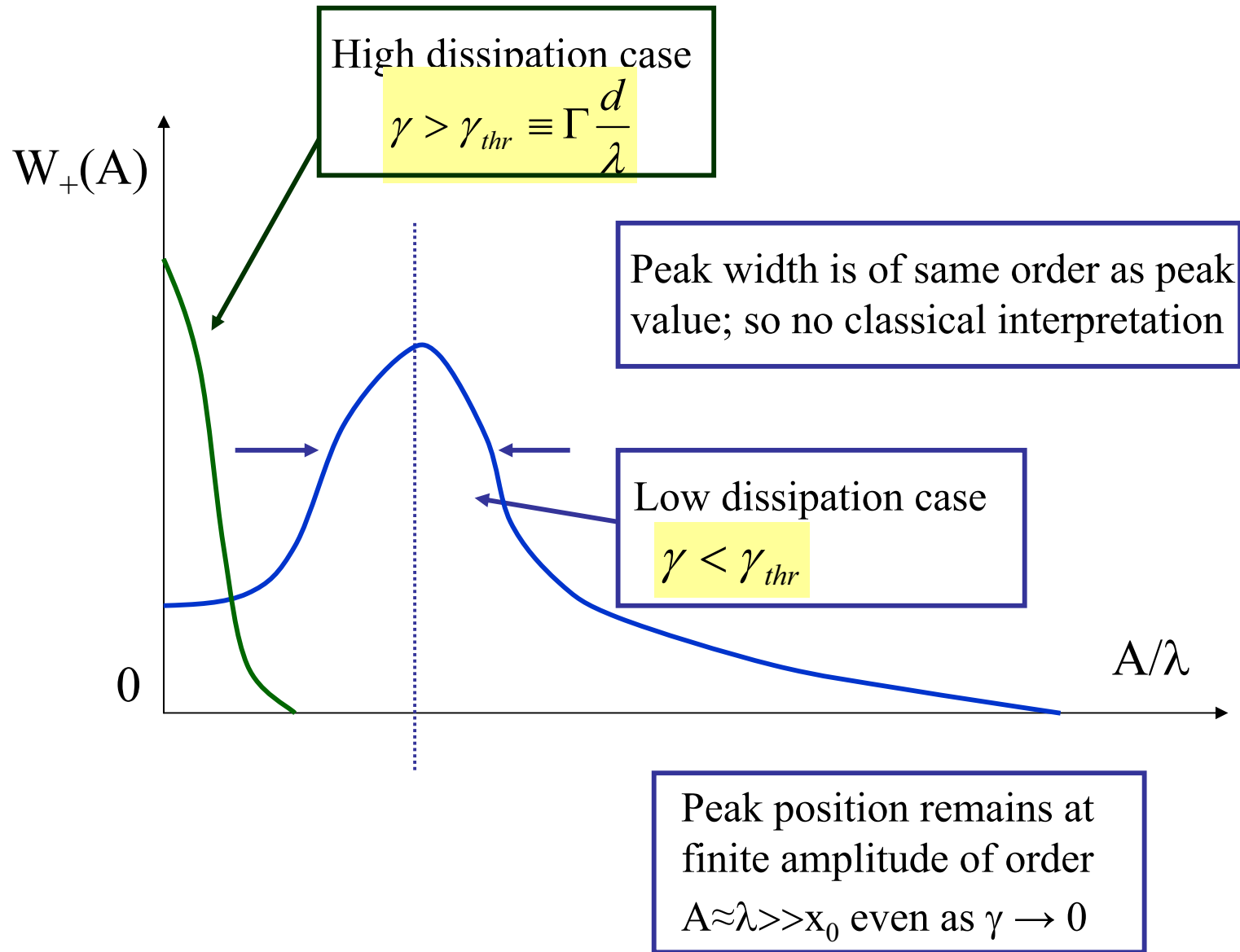
$$\hat{L}_1 \equiv \hat{L}_\gamma - \frac{\Gamma(X)}{2} \left[\cosh(\frac{i}{\lambda^2}\partial_P) - 1 \right]$$

$$\hat{L}_2 \equiv \frac{d}{\lambda}\partial_P + \frac{\Gamma(X)}{2} \left[\cosh(\frac{i}{\lambda^2}\partial_P) - 1 \right]$$

$$X \equiv \frac{x}{\lambda} ; \quad P \equiv \frac{p}{\lambda} ; \quad \Gamma_\pm(X) = \Gamma_R(X) \pm \Gamma_L(x)$$

Sketch of Results in "Classical" Regime: $E \gg E_C$

High dissipation case

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

$$W_+(A) = Tr\{\frac{1}{M\omega^2 A}\delta(\frac{1}{2}M\omega^2 A^2 - \hat{H}_\omega)\hat{\rho}_+\}$$

$$I \approx \pi \int_0^\infty dA^2 W_+(A) I_{cl}(A)$$

$W_+(A)$

A/λ

0

Width is max[d/λ,$1/\lambda^3 d$]<<1, allowing classical interpretation

Low dissipation case

Peak position same as obtained in classical description of shuttle motion, EPL 2002

Sketch of Results in "Quantum" Regime: $E << E_C$

High dissipation case

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

$W_+(A)$

Peak width is of same order as peak value; so no classical interpretation

Low dissipation case

$$\gamma < \gamma_{thr}$$

A/λ

0

Peak position remains at finite amplitude of order $A \approx \lambda >> x_0$ even as $\gamma \rightarrow 0$

Conclusions

- Electronic and mechanical degrees of freedom of nanometer-scale structures can be coupled.

- Such a coupling may result in an electro-mechanical instability and "shuttling" of electric charge (in classical and quantum regimes)
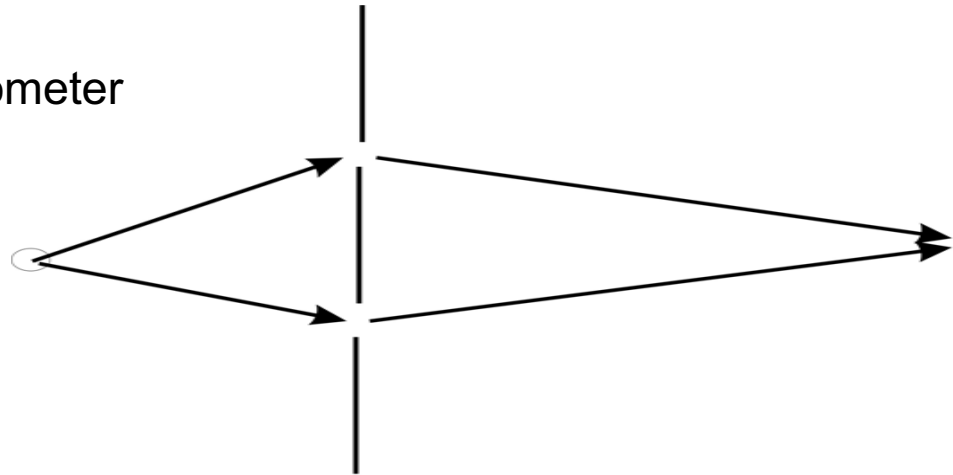
How to Detect the Quantum Nanomechanical Vibrations?

New principles should be implemented for sensing the quantum displacements
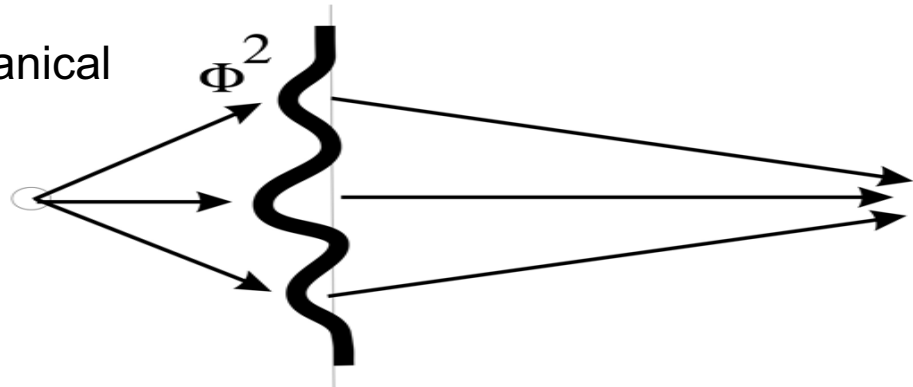
Electronic Transport Through Vibrating CNT
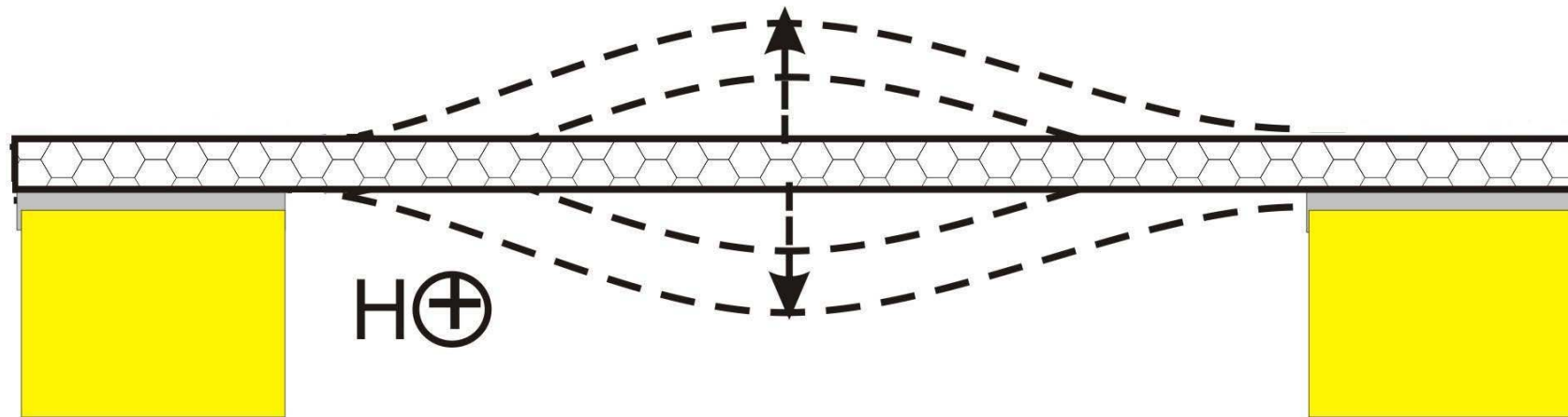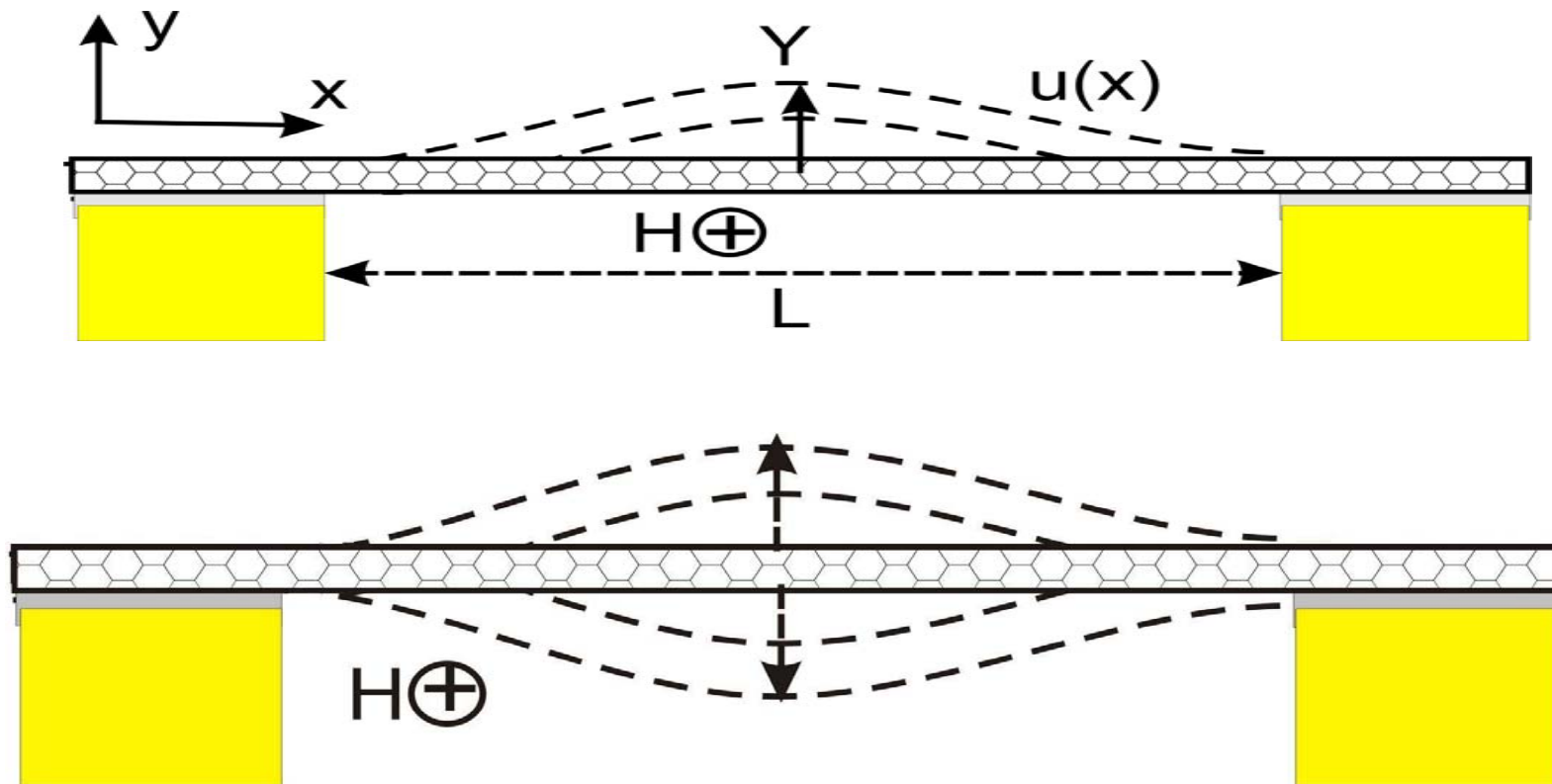
Quantum Nanomechanical Interferometer

Classical interferometer

Quantum nanomechanical
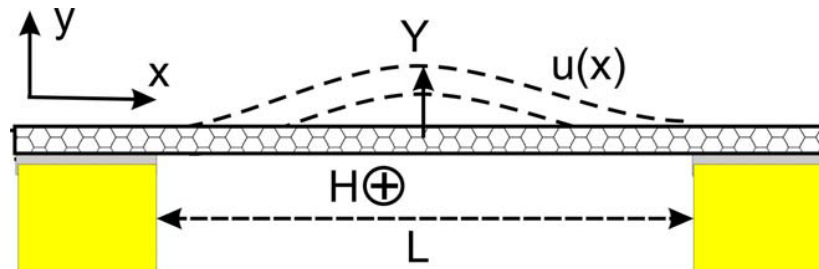interferometer

Φ^2

Classical and Quantum Vibrations

Model

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

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

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

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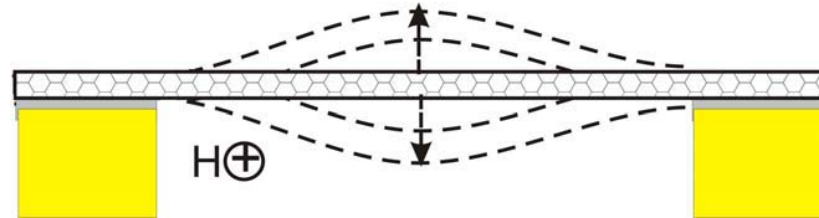
Magnetic Field Dependent Tunneling

In order to proceed it is convenient to make the unitary transformation $e^{i\hat{S}}\hat{H}e^{-i\hat{S}}$

$$\hat{S} = -i\int d^3\vec{r}\left\{\hat{u}(x)\hat{\psi}^+(\vec{r})\frac{\partial\hat{\psi}(\vec{r})}{\partial y} + i\frac{eH}{\hbar c}\left(\int_0^x dx'\hat{u}(x')\right)\hat{\psi}^+(\vec{r})\hat{\psi}(\vec{r})\right\}$$

$$\hat{H}_{el} = \int dx\hat{\psi}^+(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \varepsilon\right)\hat{\psi}(x)$$

$$\hat{H}_{mech} = \int dx\left\{\frac{1}{2\rho}[\hat{\pi}(x) - \frac{eH}{c}\int_0^x dx'\hat{\psi}^+(x')\hat{\psi}(x')]^2 + \frac{EI}{2}\left(\frac{\partial^2\hat{u}(x)}{\partial x^2}\right)^2\right\}$$

$$\hat{T}_{l/r}(H) = T\exp\left\{i\frac{eH}{\hbar c}\int_0^{\pm\frac{L}{2}} dx\hat{u}(x)\right\}\hat{T}_{l/r}(0) + h.c.$$
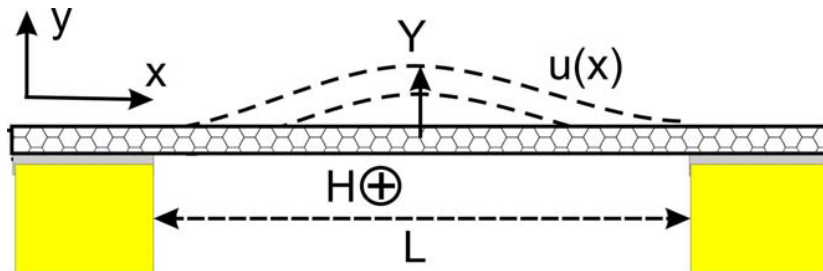
Coupling to the Fundamental Bending Mode

Only one vibration mode is taken into account

$$\hat{u}(x) = Y_0 u_0(x)(\hat{b}^+ + \hat{b}) / \sqrt{2} \; ; \quad Y_0 = \left(\hbar^2 L^2 / \beta_0 \rho E I \right)^{1/4}$$

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 Hamiltolian

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

$$\Phi = gHLY_0 / \sqrt{2}\Phi_0$$

$$Y_0 = \sqrt{\hbar/2M\omega_0} \propto \sqrt{L}$$

$$T_{eff} = T_L T_R^* \Big/ E - \mu$$

Calculation of the Electric Current

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

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

Linear Conductance

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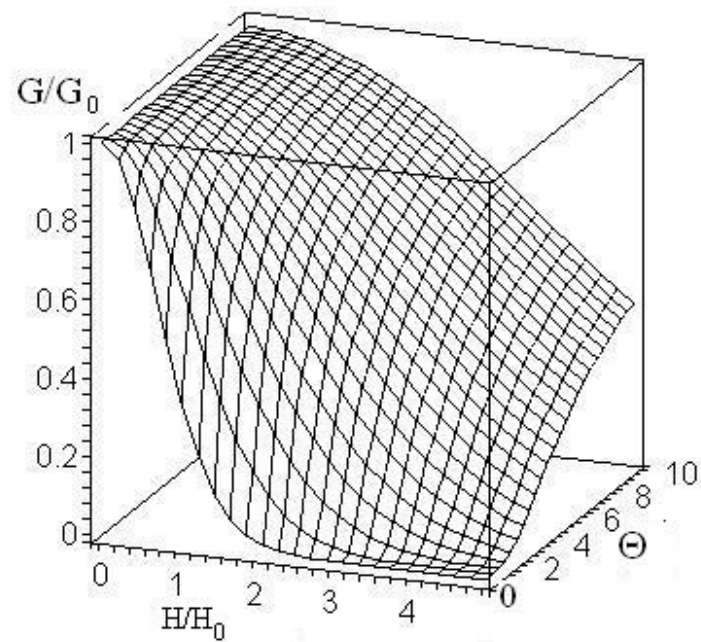
$$\frac{G}{G_0} \approx \exp\left\{-\left(\frac{\Phi}{\Phi_0}\right)^2\right\}, \quad \frac{\hbar\omega}{kT} >> 1$$

$$\frac{G}{G_0} \approx 1 - \frac{1}{6}\left(\frac{\Phi}{\Phi_0}\right)^2 \frac{\hbar\omega}{kT}, \quad \frac{\hbar\omega}{kT} << 1$$
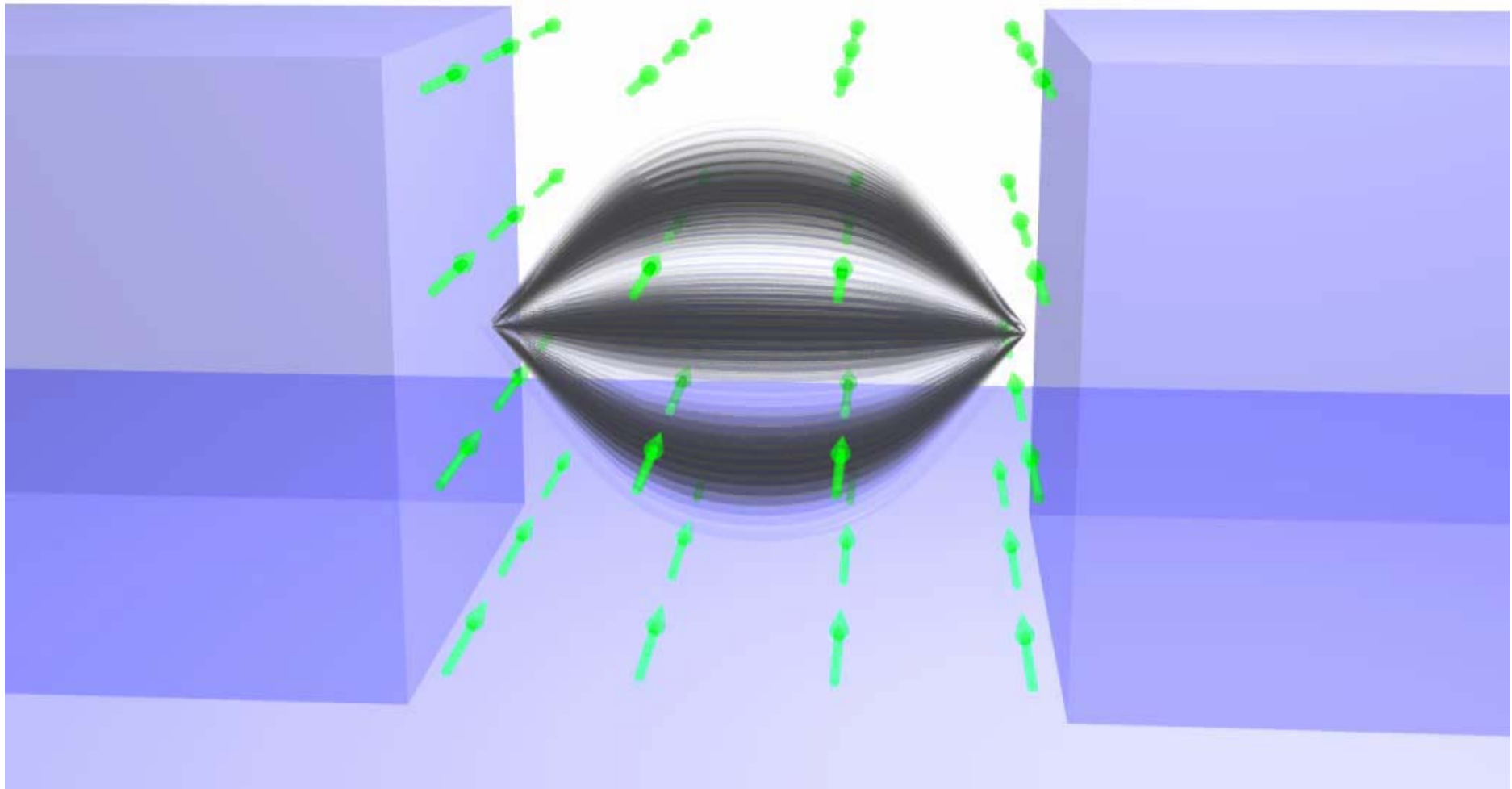
$$\Phi = 4\pi gLY_0H, \qquad \Phi_0 = \frac{hc}{e}$$

For a 1 μm long SWNT at T = 30 mK and $H \approx$ 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

- The calculations were made for a single electronic level on CNT. The generalization to continuum spectrum does not affect $G(T)/G(T=\infty)$.

- Deviation from ballisticity does not affect the result provided that $R/Ro < 10^4$

Quantum Nanoelectromechanical Coupling

- Coupling of electrons and nanomechanical vibrons form a new quantum states: ***swinging electrons***, which are responsible for current flow.

- These new states are sensitive to an external magnetic and can serve as a transducers between quantum electronic and vibronic performances.