

# Vibrational Coherences in Single Electron Tunneling through Nanoscale Oscillators

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# Outline

- 1 Model
- 2 Transport
- 3 Shot Noise

# Motivation

- Experiments with free standing nanostructures

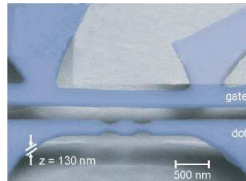


Figure: E. M. Weig *et al.*, PRL **92** 046804, (2004)

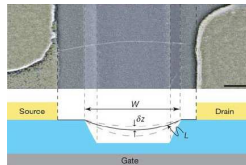
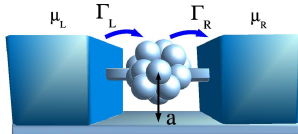


Figure: V. Sazanova *et al.*, Nature **431** 284, (2004)



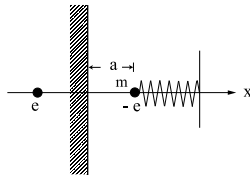
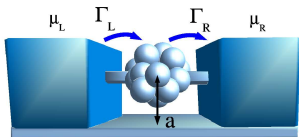
# Model

Single electron transport through a vibrating Quantum Dot



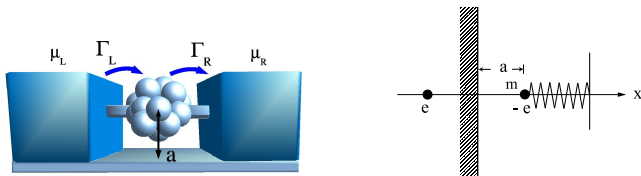
# Model

Single electron transport through a vibrating Quantum Dot



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Single electron transport through a vibrating Quantum Dot



$$H = \frac{\mathbf{P}^2}{2m} + \frac{1}{2}m\omega_0^2(\mathbf{a} - \mathbf{r})^2 - d^\dagger d \frac{e^2}{4\pi\epsilon_0} \frac{1}{2\mathbf{r} \cdot \mathbf{n}} \quad (1)$$

dot creation and annihilation operators;

$$d^\dagger = |1\rangle_{el} \langle 0|_{el} \quad d = |0\rangle_{el} \langle 1|_{el}. \quad (2)$$

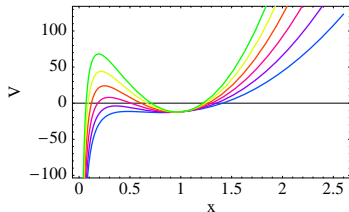
Eigenstates  $|n, \nu\rangle = |n\rangle_{vib} \otimes |\nu\rangle_{el}$

## Superposition of Hydrogen atom and harmonic oscillator

$$H = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{\Omega^2}{2} (1-x)^2 - \frac{\epsilon}{x} \quad (3)$$

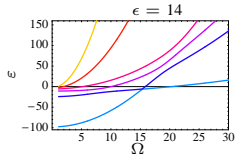
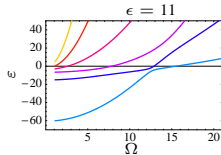
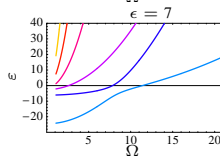
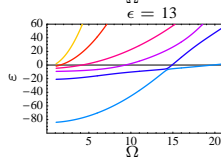
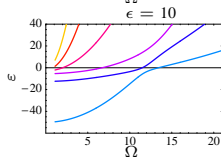
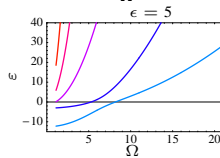
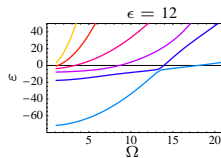
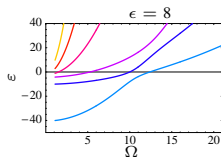
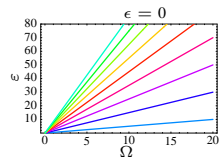
where

$$\frac{x}{a} \rightarrow x \quad , \quad \frac{1}{\hbar^2} m^2 \omega_0^2 a^4 \rightarrow \Omega^2 \quad , \quad \frac{ame^2}{8\hbar^2 \pi \epsilon_0} \rightarrow \epsilon \quad (4)$$

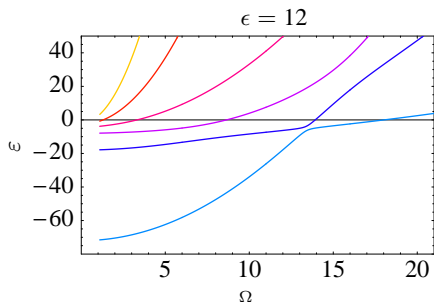




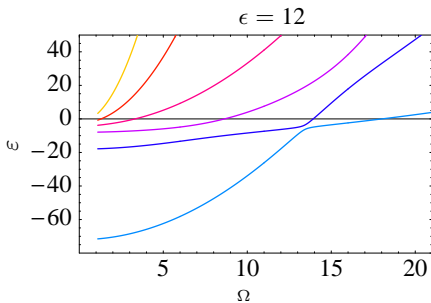
## Spectrum



- Consider  $\epsilon = 12$



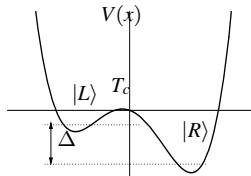
- Consider  $\epsilon = 12$



- Effective Two-Level-System at  $\Omega \approx 13$

Why two level system?

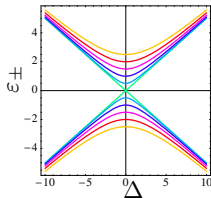
$$H = \begin{pmatrix} \frac{\Delta}{2} & T_c \\ T_c & -\frac{\Delta}{2} \end{pmatrix}$$



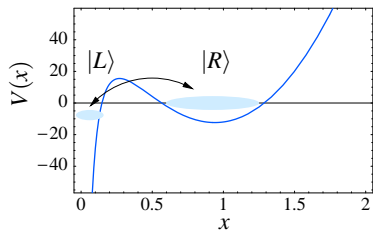
Eigensystem:

$$\epsilon_{\pm} = \pm \frac{1}{2} \sqrt{\Delta^2 + 4T_c^2} \quad (5)$$

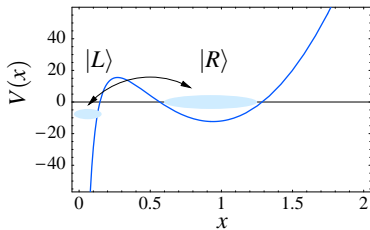
$$|\pm\rangle = \alpha |L\rangle \pm \beta |R\rangle \quad (6)$$



→ coherent tunneling of vibrational states

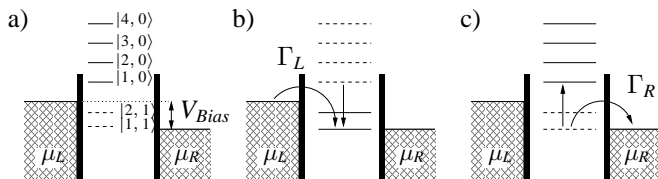


→ coherent tunneling of vibrational states



How can we measure this?

# Transport



$$H = H_{\text{Dot}} + H_{\text{Res}} + H_{\text{T}} \quad (7)$$

Eigenstates of  $H_{\text{Dot}}$  are denoted as  $|n, \nu\rangle = |n\rangle_{\text{vib}} \otimes |\nu\rangle_{\text{el}}$ .

$$H_{\text{Dot}} = \sum_{i,j} \varepsilon_{1,i} |i, 1\rangle \langle i, 1| + \varepsilon_{0,j} |j, 0\rangle \langle j, 0| \quad (8)$$

$$H_{\text{Res}} = \sum_{k,L,R} \varepsilon_k c_k^\dagger c_k \quad (9)$$

$$H_{\text{T}} = \sum_{k,L,R} T_k (c_k^\dagger d + d^\dagger c_k) \quad (10)$$

# Master equation

Liouville-von Neumann equation in interaction picture

$$\dot{\tilde{\chi}}(t) = -i[\tilde{H}_T(t), \tilde{\chi}(t)]. \quad (11)$$



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$$\dot{\tilde{\chi}}(t) = -i[\tilde{H}_T(t), \tilde{\chi}(t)]. \quad (11)$$

Tracing out the reservoirs and expanding the commutators yields to second order

$$\begin{aligned} \dot{\tilde{\rho}}(t) = & - \sum_{k_{L,R}} \int_0^t dt' |T_k|^2 f(\varepsilon_k) e^{i\varepsilon_k(t-t')} [\tilde{d}(t) \tilde{d}^\dagger(t') \tilde{\rho}(t') - \tilde{d}^\dagger(t') \tilde{\rho}(t') \tilde{d}(t)] \\ & - \sum_{k_{L,R}} \int_0^t dt' |T_k|^2 (1 - f(\varepsilon_k)) e^{-i\varepsilon_k(t-t')} [\tilde{d}^\dagger(t) \tilde{d}(t') \tilde{\rho}(t') - \tilde{d}(t') \tilde{\rho}(t') \tilde{d}^\dagger(t)] \\ & - \sum_{k_{L,R}} \int_0^t dt' |T_k|^2 f(\varepsilon_k) e^{-i\varepsilon_k(t-t')} [\tilde{\rho}(t') \tilde{d}(t') \tilde{d}^\dagger(t) - \tilde{d}^\dagger(t) \tilde{\rho}(t') \tilde{d}(t')] \\ & - \sum_{k_{L,R}} \int_0^t dt' |T_k|^2 (1 - f(\varepsilon_k)) e^{i\varepsilon_k(t-t')} [\tilde{\rho}(t') \tilde{d}^\dagger(t') \tilde{d}(t) - \tilde{d}(t) \tilde{\rho}(t') \tilde{d}^\dagger(t')] \end{aligned} \quad (12)$$

Matrix elements, Markov approximation ( $\tilde{\rho}(t') \rightarrow \tilde{\rho}(t)$ ) and transform into Schrödinger picture:

$$\begin{aligned}
 \frac{d}{dt} \langle n, \nu | \rho(t) | m, \mu \rangle = & -i(\varepsilon_{\nu n} - \varepsilon_{\mu m}) \langle n, \nu | \rho_t | m, \mu \rangle - \\
 & - \sum_{\alpha=L,R} \sum_{i,j,i',j'} \{ \gamma_{\alpha}(\varepsilon_{1i} - \varepsilon_{0j'}) \tau_{in} \tau_{ij'} \langle j', 0 | \rho_t | m, \mu \rangle \delta_{\nu 0} \\
 & - \gamma_{\alpha}(\varepsilon_{1n} - \varepsilon_{0j}) \tau_{nj} \tau_{mj'} \langle j, 0 | \rho_t | j', 0 \rangle \delta_{\nu 1} \delta_{\mu 1} + \\
 & + \bar{\gamma}_{\alpha}(\varepsilon_{1i'} - \varepsilon_{0j}) \tau_{nj} \tau_{i'j} \langle i', 1 | \rho_t | m, \mu \rangle \delta_{\nu 1} - \\
 & - \bar{\gamma}_{\alpha}(\varepsilon_{1i} - \varepsilon_{0n}) \tau_{in} \tau_{i'm} \langle i, 1 | \rho_t | i', 1 \rangle \delta_{\nu 0} \delta_{\mu 0} + \\
 & + \gamma_{\alpha}(\varepsilon_{1i'} - \varepsilon_{0j}) \tau_{i'j} \tau_{i'm} \langle n, \nu | \rho_t | j, 0 \rangle \delta_{\mu 0} - \\
 & - \gamma_{\alpha}(\varepsilon_{1m} - \varepsilon_{0j'}) \tau_{nj} \tau_{mj'} \langle j, 0 | \rho_t | j', 0 \rangle \delta_{\nu 1} \delta_{\mu 1} + \\
 & + \bar{\gamma}_{\alpha}(\varepsilon_{1i} - \varepsilon_{0j'}) \tau_{ij'} \tau_{mj'} \langle n, \nu | \rho_t | i, 1 \rangle \delta_{\mu 1} - \\
 & - \bar{\gamma}_{\alpha}(\varepsilon_{1i'} - \varepsilon_{0m}) \tau_{in} \tau_{i'm} \langle i, 1 | \rho_t | i', 1 \rangle \delta_{\nu 0} \delta_{\mu 0} \} \quad (13)
 \end{aligned}$$

# Franck-Condon principle

The  $\tau_{ij}$  are the Franck-Condon factors

$$\tau_{ij} = {}_1\langle i|j\rangle_0 = \int_0^\infty \psi_{1,i}(x)\psi_{0,j}(x) \quad (14)$$

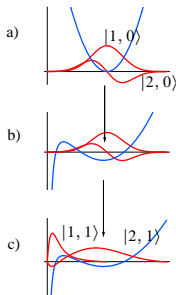
overlap of the vibrational wavefunctions before and after an electronic transition

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# Current

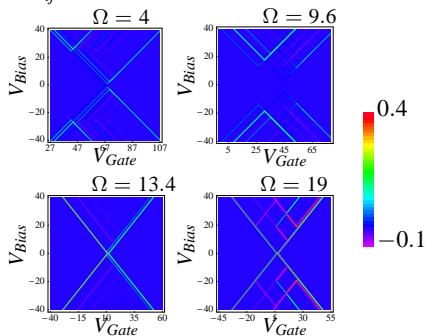
Rates  $\gamma_\alpha(\varepsilon) = \Gamma_\alpha f_\alpha(\varepsilon)$  for tunnelling onto the dot and  $\bar{\gamma}_\alpha(\varepsilon) = \Gamma_\alpha(1 - f_\alpha(\varepsilon))$  for tunnelling off the dot.

$$\langle I \rangle = - \sum_{ij} e(\gamma^L(\varepsilon_{1i} - \varepsilon_{0j})\rho_{i_1 i_1} - \bar{\gamma}^L(\varepsilon_{1i} - \varepsilon_{0j})\rho_{j_0 j_0}) \quad (15)$$

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→ Franck-Condon blockade (nice), but where is the oscillation?

# Shot Noise

- Current as a series of single electron transistions

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- Genrally: insight to internal dynamics, just as current
- Defined from current-current correlation

$$S(\omega) = \int_{-\infty}^{\infty} d\tau e^{i\omega\tau} \langle [\Delta I(t), \Delta I(t + \tau)]_+ \rangle \quad (16)$$

where  $\Delta I(t) = I(t) - \langle I \rangle$

# Superoperators

- Master equation as a Liouvillian superoperator

$$\dot{\rho}(t) = \mathcal{L}\rho(t) = (\mathcal{L}_0 + \mathcal{L}_J)\rho(t) \quad (17)$$

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$$S(\omega) = \langle\langle 0 | \mathcal{L}_J | 0 \rangle\rangle - 2\text{Re}[\langle\langle 0 | \mathcal{L}_J \mathcal{R}(\omega) \mathcal{L}_J | 0 \rangle\rangle] \quad (19)$$

where  $\mathcal{R}(\omega)$  is the pseudo inverse of  $(i\omega - \mathcal{L})$



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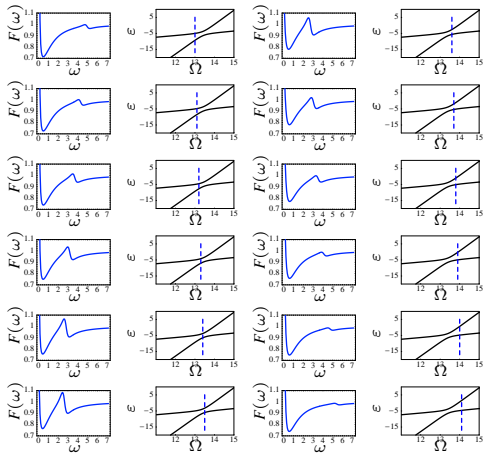
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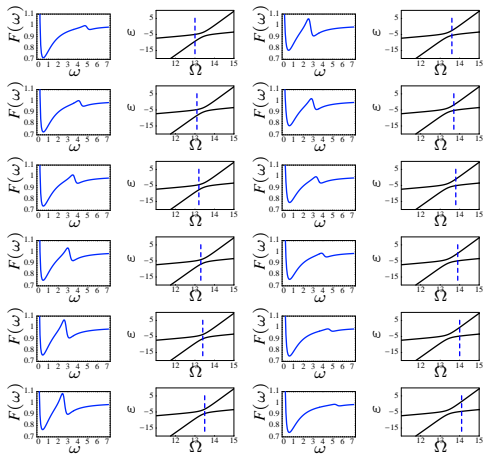
$$S(\omega) = \langle\langle 0 | \mathcal{L}_J | 0 \rangle\rangle - 2\text{Re}[\langle\langle 0 | \mathcal{L}_J \mathcal{R}(\omega) \mathcal{L}_J | 0 \rangle\rangle] \quad (19)$$

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- Fano factor

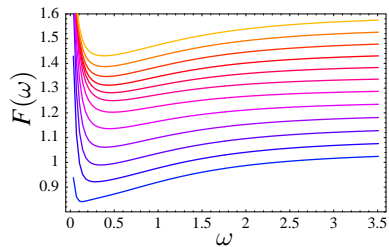
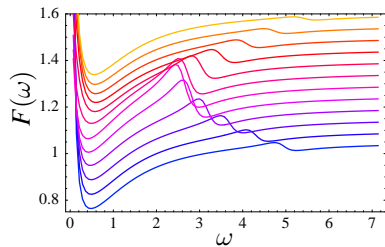
$$F(\omega) = \frac{S(\omega)}{\langle I \rangle} \quad (20)$$



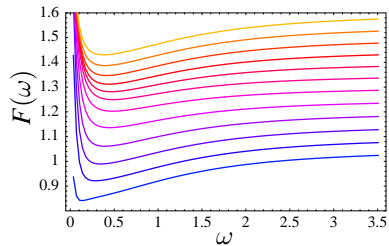
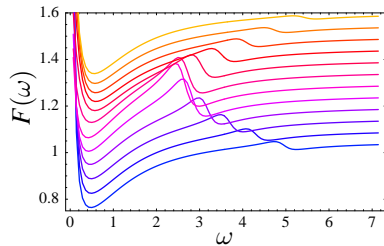


→ coherent tunneling of the vibrational state.

Comparison with a rate equation approach using Fermis Golden Rule:



Comparison with a rate equation approach using Fermis Golden Rule:



→ Keeping the coherences is crucial for this feature.

# Conclusion

- Model for single electron transport through vibrating quantum dot with Image charge
- Two level system points to coherent oscillations
- Franck-Condon Master equation
- Coherent interaction visible in noise spectrum due to coherences in master equation

Thank you very much!!

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Lets go to lunch!!