



**The Abdus Salam
International Centre for Theoretical Physics**



1957-26

Miniworkshop on Strong Correlations in Materials and Atom Traps

4 - 15 August 2008

Novel Gutzwiller Approach to the Kondo lattice

SCHIRO' Marco and FABRIZIO Michele

*S.I.S.S.A.
International School for Advanced Studies
Via Beirut 2-4
34014 Trieste
Italy*

Real-Time Diagrammatic Monte Carlo for Non-Equilibrium Quantum Transport

Marco Schirò¹ and **Michele Fabrizio^{1,2}**

¹SISSA and Democritos

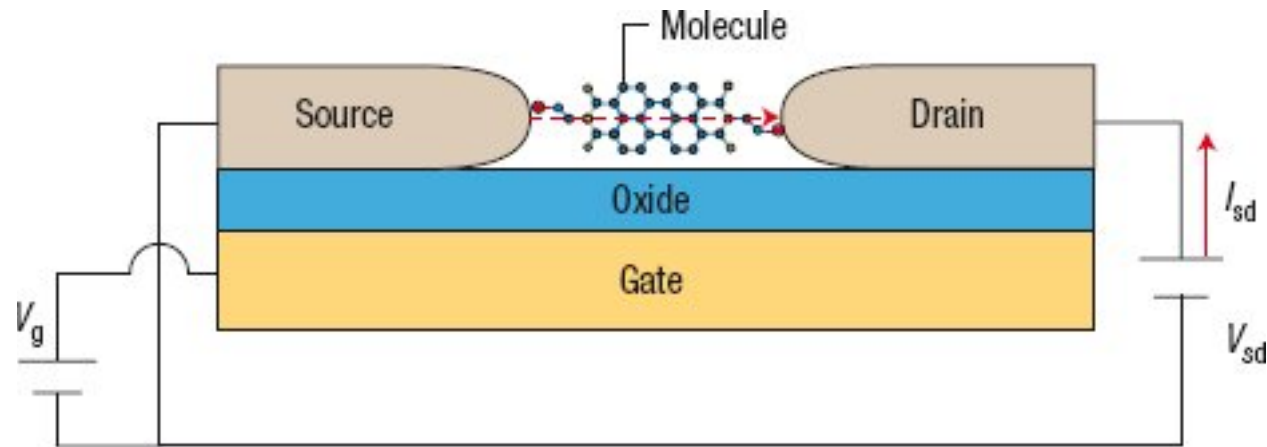
²ICTP



DEMOCRITOS
DEmocritos MOdeling Center for
Research In aTOMistic Simulation **INFM**

Motivations: Quantum Transport at Nanoscale

Experiments start to measure non equilibrium transport through small quantum objects, like atoms or small molecules → **Single-Molecule Electronics is coming!**

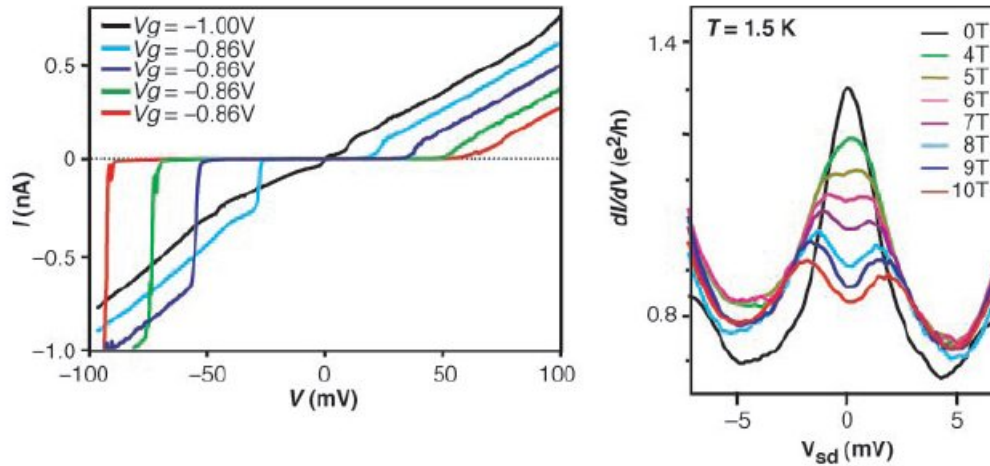


N.J.Tao, Nature Nanotechnology (2006)

Ingredients for new physics

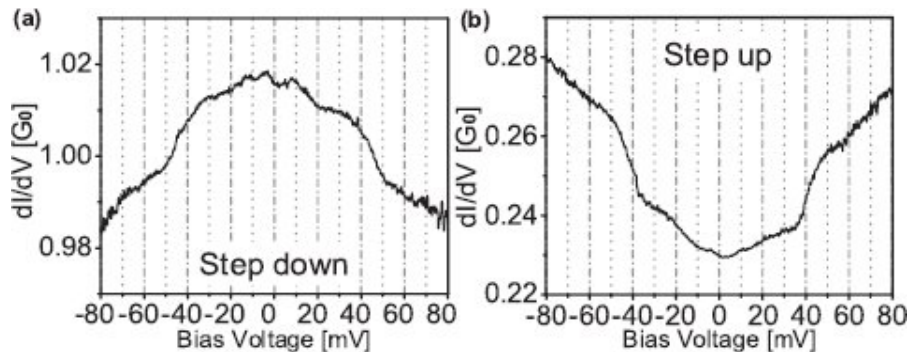
- ▶ Interplay **Non-Equilibrium/Strong Correlations**
- ▶ Coupling to **Molecular Vibrations**
- ▶ **Superconducting Leads**

Motivations: Quantum Transport at Nanoscale



Park *et al.*, Nature (2000)

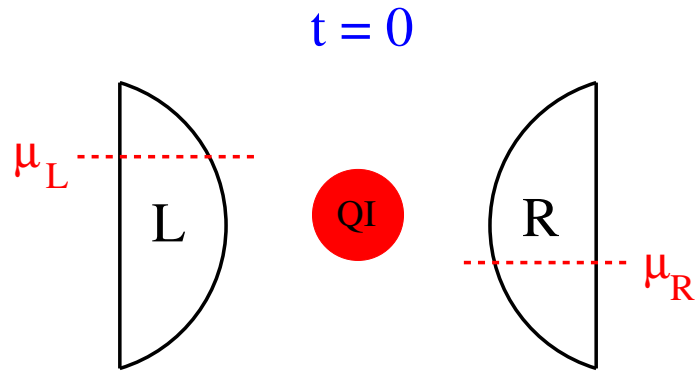
Kondo Physics!



Tal, Krieger *et al.* PRL (08)

Electron-Vibron Coupling

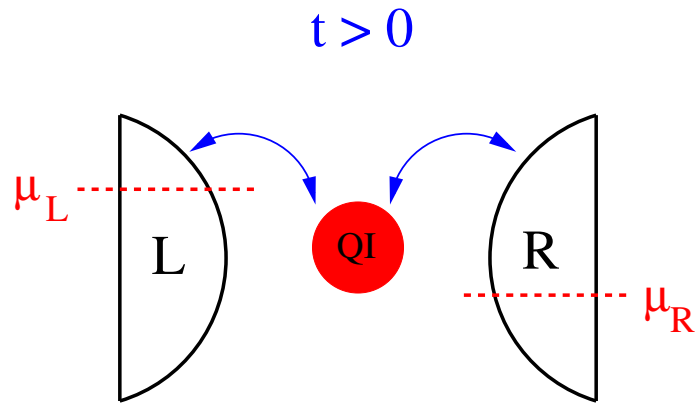
Modeling Non Equilibrium Transport through Nanodevices



$$H_0 = \sum_{k, \alpha=L, R} \xi_{k\alpha} f_{k\alpha}^\dagger f_{k\alpha} + H_{loc}[c^\dagger, c]$$

$$\rho(t=0) = \rho_{Leads} \otimes \rho_{loc}$$

Modeling Non Equilibrium Transport through Nanodevices



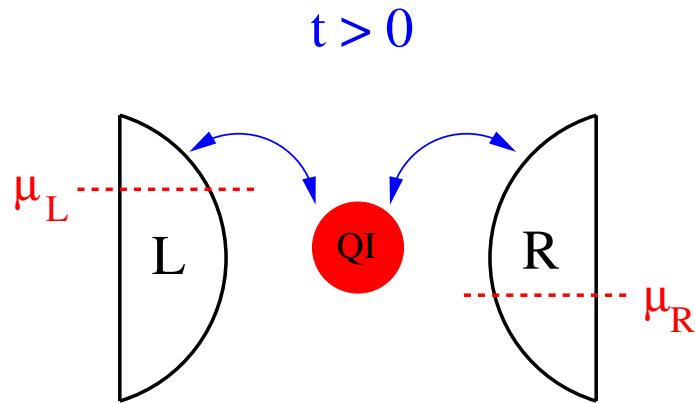
$$H(t > 0) = H_0 + \sum_{k\alpha} V_{k\alpha} (f_{k\alpha}^\dagger c + c^\dagger f_{k\alpha})$$

$$\rho(t) = U^\dagger(t) \rho_0 U(t)$$

$$\langle I(t) \rangle = \text{Tr}[\rho_0 I(t)] \quad I(t) = T e^{i \int_0^t d\tau H(\tau)} I \tilde{T} e^{i \int_0^t d\tau H(\tau)}$$

- ▶ $\mu_L \neq \mu_R \longrightarrow$ Non-Equilibrium Steady-State, Dissipation
- ▶ Main Goal: Compute $I - V$, dI/dV , d^2I/dV^2 in the steady-state
- ▶ Equilibrium methods are ruled out: **Real-Time Dynamics is the challenge!**

Modeling Non Equilibrium Transport through Nanodevices



$$H(t > 0) = H_0 + \sum_{k\alpha} V_{k\alpha} (f_{k\alpha}^\dagger c + c^\dagger f_{k\alpha})$$

$$\rho(t) = U^\dagger(t) \rho_0 U(t)$$

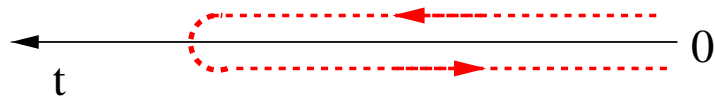
$$\langle I(t) \rangle = \text{Tr}[\rho_0 I(t)] \quad I(t) = T e^{i \int_0^t d\tau H(\tau)} I \tilde{T} e^{i \int_0^t d\tau H(\tau)}$$

Theoretical Approaches

- ▶ Keldysh Perturbation Theory \implies Konig&Schoeller (2000)
- ▶ Time-dependent NRG \implies Anders&Schiller (2006)
- ▶ Diagrammatic Monte Carlo on the Keldysh Contour \implies **This Talk!**

Keldysh Diagrammatic Monte Carlo

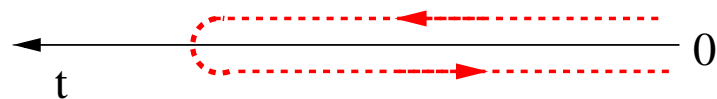
- ▶ Monte Carlo Sampling of Keldysh Perturbation Theory in H_{tun}



$$\langle O(t) \rangle = \text{Tr} \rho_0 T_K \left(e^{i \int_K d\tau H_0 + H_{tun}} O \right)$$

Keldysh Diagrammatic Monte Carlo

- ▶ Monte Carlo Sampling of Keldysh Perturbation Theory in H_{tun}



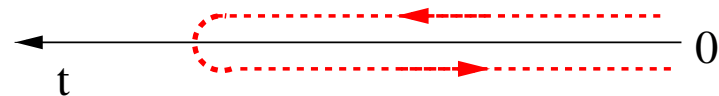
A Keldysh contour diagram in the time domain. A solid horizontal line starts at time t on the left and ends at time 0 on the right. A dashed horizontal line starts at time 0 on the left and ends at time t on the right. A small semi-circular dashed line connects the two horizontal lines at time 0 . Red arrows on the dashed line point from right to left, and red arrows on the solid line point from left to right.

$$\langle O(t) \rangle = \text{Tr} \rho_0 T_K \left(e^{i \int_K d\tau H_0 + H_{tun}} O \right)$$

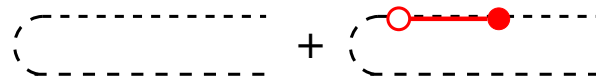
$$\langle n(t) \rangle = \text{---}$$

Keldysh Diagrammatic Monte Carlo

- ▶ Monte Carlo Sampling of Keldysh Perturbation Theory in H_{tun}

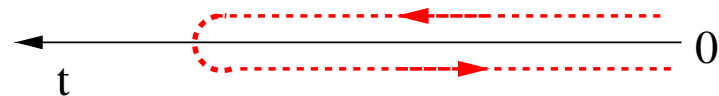


$$\langle O(t) \rangle = \text{Tr} \rho_0 T_K \left(e^{i \int_K d\tau H_0 + H_{tun}} O \right)$$

$$\langle n(t) \rangle = \text{Diagram 1} + \text{Diagram 2}$$


Keldysh Diagrammatic Monte Carlo

- ▶ Monte Carlo Sampling of Keldysh Perturbation Theory in H_{tun}

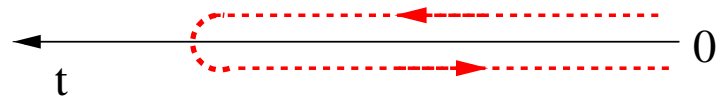


$$\langle O(t) \rangle = Tr \rho_0 T_K \left(e^{i \int_K d\tau H_0 + H_{tun}} O \right)$$

$$\langle n(t) \rangle = \text{[diagram 1]} + \text{[diagram 2]}$$


Keldysh Diagrammatic Monte Carlo

- ▶ Monte Carlo Sampling of Keldysh Perturbation Theory in H_{tun}

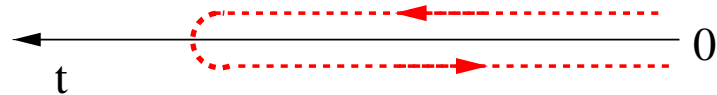


$$\langle O(t) \rangle = \text{Tr} \rho_0 T_K \left(e^{i \int_K d\tau H_0 + H_{tun}} O \right)$$

$$\langle n(t) \rangle = \text{---} + \text{---} \text{---} \text{---}$$

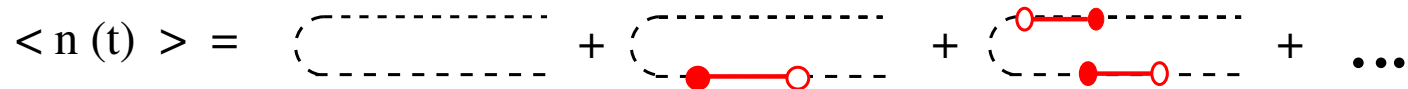

Keldysh Diagrammatic Monte Carlo

- ▶ Monte Carlo Sampling of Keldysh Perturbation Theory in H_{tun}



A Keldysh contour diagram in the time domain. A horizontal axis labeled 't' has an arrow pointing to the left. A solid line starts at a point labeled '0' on the right and extends to the left. A dashed red line branches off from the solid line, goes up, then left, then down, and then back to the right, forming a loop. Red arrows on the dashed line indicate a clockwise direction of integration.

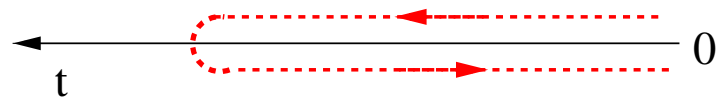
$$\langle O(t) \rangle = Tr \rho_0 T_K \left(e^{i \int_K d\tau H_0 + H_{tun}} O \right)$$

$$\langle n(t) \rangle = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots$$



A series of diagrams representing the expansion of the average number of particles $\langle n(t) \rangle$. Each diagram consists of a dashed black loop. The first diagram is a simple dashed loop. The second diagram has a solid red line segment at the bottom with a red filled circle on the left and a red open circle on the right. The third diagram has two solid red line segments at the bottom, each with a red filled circle on the left and a red open circle on the right. The series ends with an ellipsis.

Keldysh Diagrammatic Monte Carlo

- ▶ Monte Carlo Sampling of Keldysh Perturbation Theory in H_{tun}

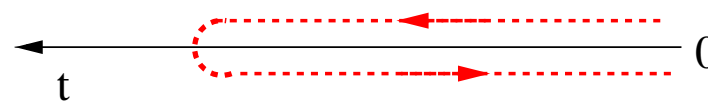


$$\langle O(t) \rangle = \text{Tr} \rho_0 T_K \left(e^{i \int_K d\tau H_0 + H_{tun}} O \right)$$

$$\langle n(t) \rangle = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots$$


Keldysh Diagrammatic Monte Carlo

- ▶ Monte Carlo Sampling of Keldysh Perturbation Theory in H_{tun}



$$\langle O(t) \rangle = Tr \rho_0 T_K \left(e^{i \int_K d\tau H_0 + H_{tun}} O \right)$$

$$\langle n(t) \rangle = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots$$

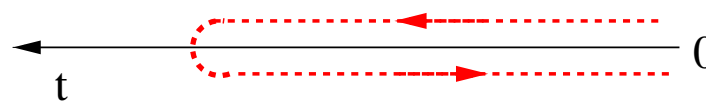
The diagrams show a dashed rectangular contour. The first is empty. The second has a red solid line segment on the bottom edge with a red dot at its left end and an open red circle at its right end. The third has a red solid line segment on the top edge with an open red circle at its left end and a red dot at its right end.

$$\langle n(t) \rangle = \sum_{n=0}^{\infty} \int det \Delta_{leads}(t_1^e, \dots, t_n^e | t_1^s, \dots, t_n^s) \langle T_K \{ c(t_1^e) c^\dagger(t_1^s) \dots c(t_n^e) c^\dagger(t_n^s) n(t) \} \rangle_{loc}$$

- ▶ Basic MC Updates: Adding/Removing/Shifting segments on the contour

Keldysh Diagrammatic Monte Carlo

- ▶ Monte Carlo Sampling of Keldysh Perturbation Theory in H_{tun}



$$\langle O(t) \rangle = \text{Tr} \rho_0 T_K \left(e^{i \int_K d\tau H_0 + H_{tun}} O \right)$$

$$\langle n(t) \rangle = \text{[diagram 1]} + \text{[diagram 2]} + \text{[diagram 3]} + \dots$$

The diagrams show a dashed contour with various red segments and dots representing interaction terms.

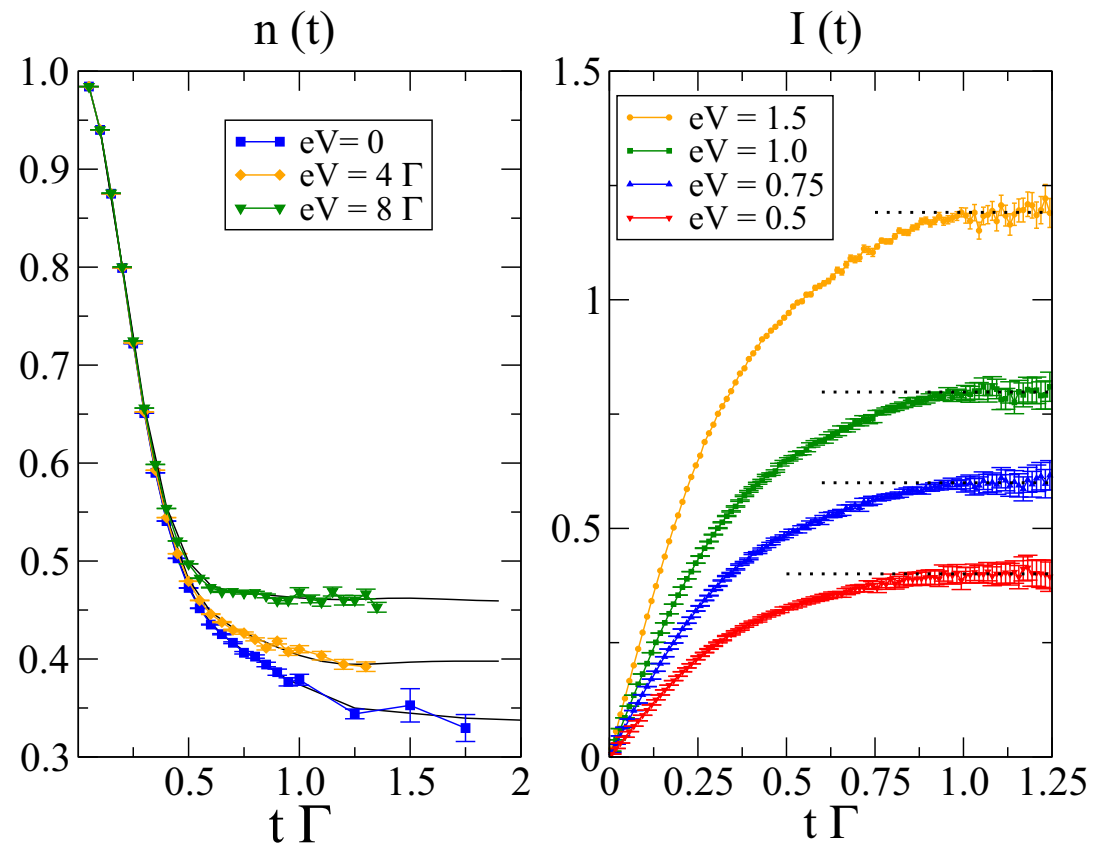
$$\langle n(t) \rangle = \sum_{n=0}^{\infty} \int \det \Delta_{leads}(t_1^e, \dots, t_n^e | t_1^s, \dots, t_n^s) \langle T_K \{ c(t_1^e) c^\dagger(t_1^s) \dots c(t_n^e) c^\dagger(t_n^s) n(t) \} \rangle_{loc}$$

- ▶ Basic MC Updates: Adding/Removing/Shifting segments on the contour

Summing-Up K-diagMC:

1. Non-Perturbative approach to Real-Time Dynamics
2. Numerically Exact: no truncation in the bath/dynamics
3. Sign Problem is a critical issue!

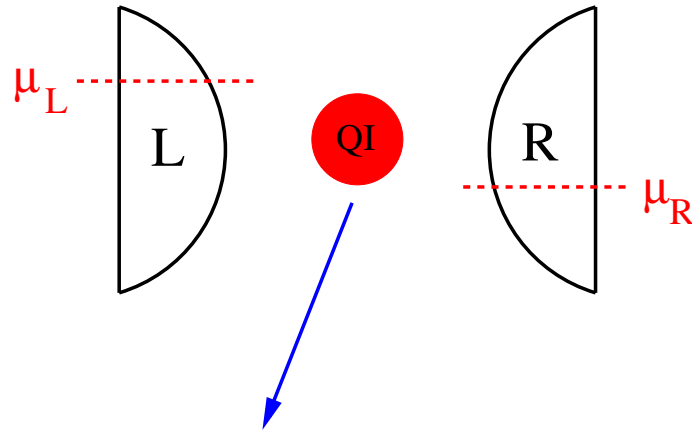
Benchmark: Biased Resonant Level Model



Lesson from a simple case:

1. **Great accuracy** on the relevant time scale $t \sim 1/\Gamma$
2. Dissipation occurs entirely within the fermionic reservoirs

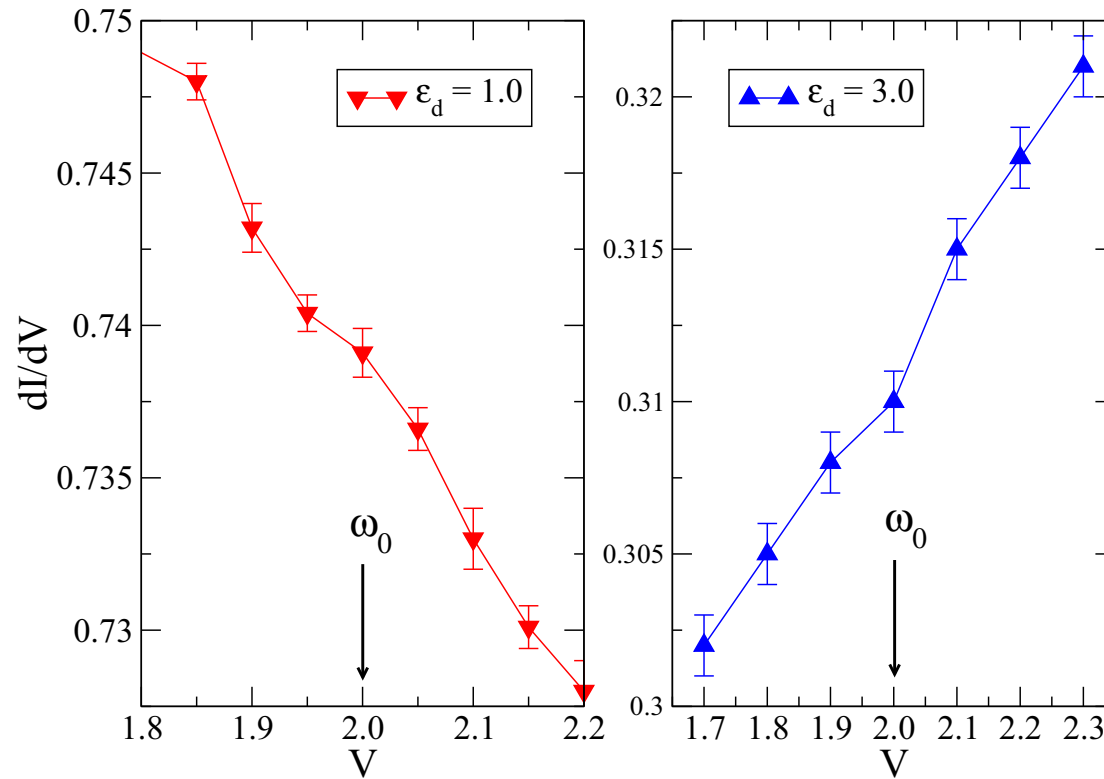
Non-Equilibrium Transport through a single molecule



$$H_{loc}(n) = \frac{\omega_0}{2}(x^2 + p^2) + gx(n - \frac{1}{2}) + \epsilon_d(n - \frac{1}{2})$$

- ▶ Electron-Vibron Coupling affects dI/dV spectrum
- ▶ Perturbation Theory predicts sharp jump in dI/dV at $eV \simeq \hbar\omega_0$

Non-Equilibrium Transport through a single molecule



- ▶ Step-Down to Step-Up crossover!
- ▶ Non-Perturbative effects act to broaden the feature

Conclusions and Outlooks

Quantum Transport through Molecular Conductors is challenging

- ▶ Rich new physics is expected when local interacting degrees of freedom are driven out of equilibrium
- ▶ New non-perturbative methods are needed

Diagrammatic MC on the Keldysh Contour looks promising:

- ▶ Novel approach to Non-Equilibrium Transport \mapsto Current, Conductance
- ▶ No finite-size effects in the bath or in the dynamics
- ▶ Case Study: Inelastic Tunneling Spectra for a single-molecule conductor