The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

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

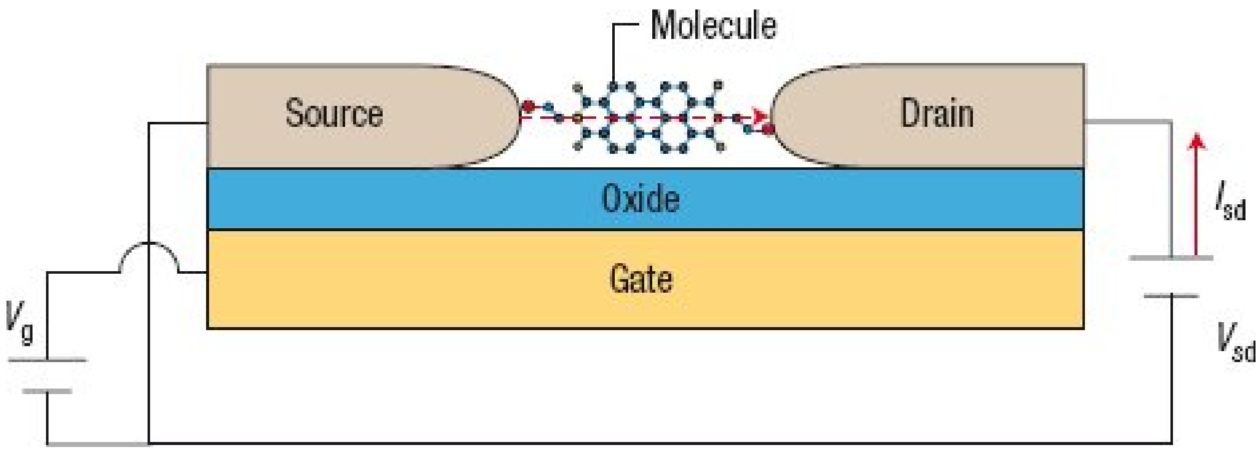
Marco Schirò[1] and Michele Fabrizio[1,2]

[1]SISSA and Democritos

[2]ICTP

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!

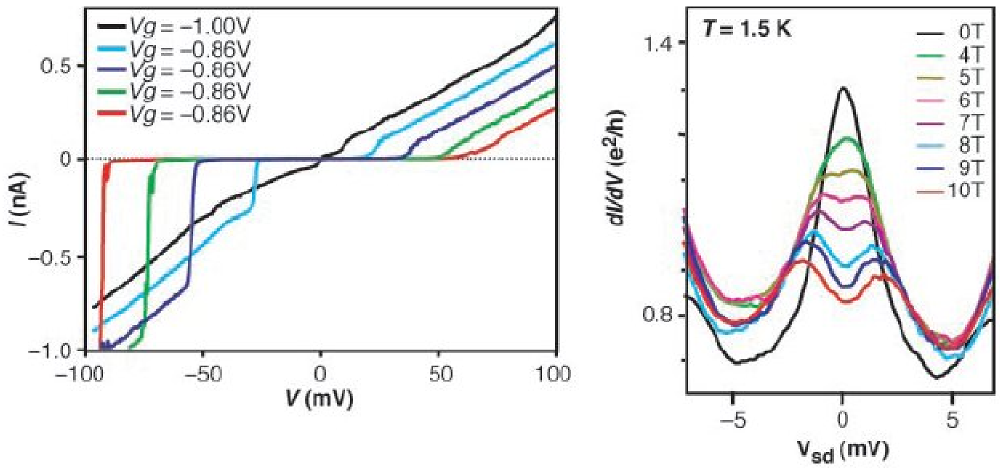


N.J.Tao, Nature Nanotechnology (2006)

Ingredients for new physics

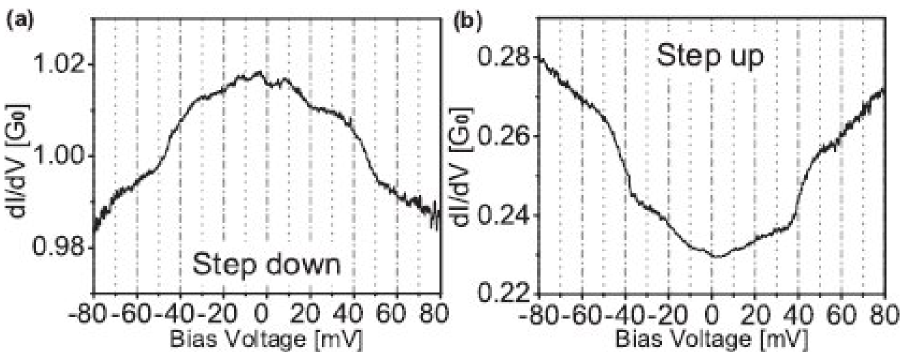
- Interplay Non-Equilibrium/Strong Correlations
- Coupling to Molecular Vibrations
- Superconducting Leads

Motivations: Quantum Transport at Nanoscale



Park *et al.*, Nature (2000)

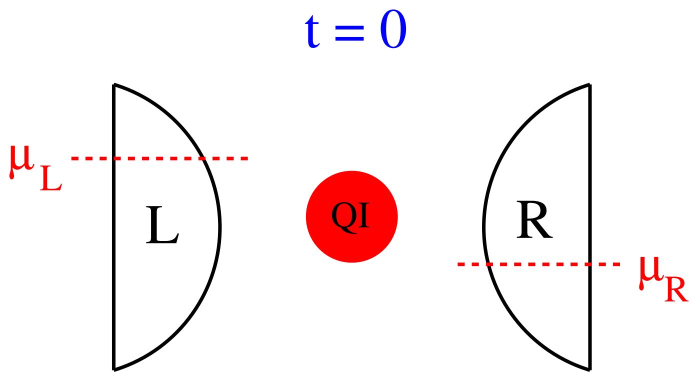
Kondo Physics!



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

Electron-Vibron Coupling

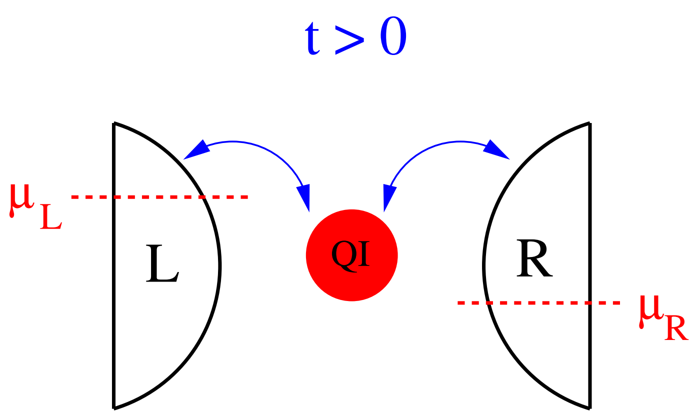
Modeling Non Equilibrium Transport through Nanodevices



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

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

Modeling Non Equilibrium Transport through Nanodevices



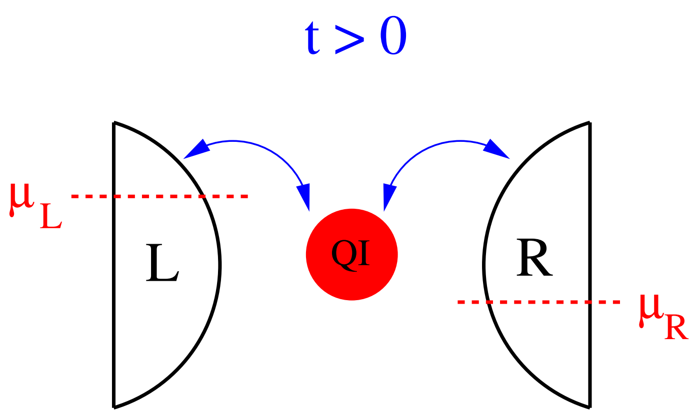
$$H(t>0) = H_0 + \sum_{k\alpha} V_{k\alpha}\left(f^\dagger_{k\alpha} c + c^\dagger f_{k\alpha}\right)$$

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

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

- $\mu_L \neq \mu_R \longmapsto$ 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



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

$$\rho(t) = U^{\dagger}(t)\,\rho_0\,U(t)$$

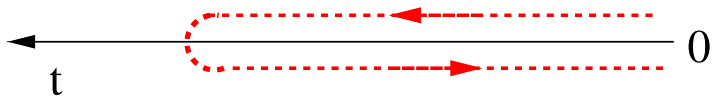
$$\langle I(t)\rangle = Tr\left[\rho_0 I(t)\right] \qquad I(t) = T\,e^{i\int_0^t d\tau H(\tau)}\, I\, \tilde{T}\, e^{i\int_0^t d\tau H(\tau)}$$

Theoretical Approaches

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

Keldysh Diagrammatic Monte Carlo

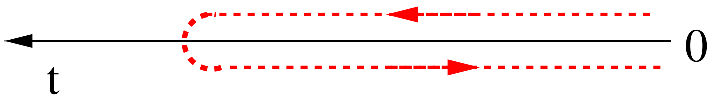
- Monte Carlo Sampling of Keldysh Perturbation Theory in H_{tun}



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

Keldysh Diagrammatic Monte Carlo

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

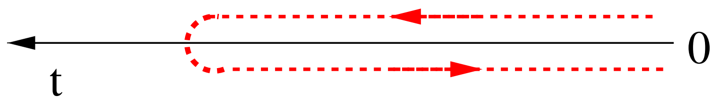


$$\langle O(t)\rangle = Tr\,\rho_0\,T_K\left(e^{i\int_K d\tau\, H_0+H_{tun}}\,O\right)$$

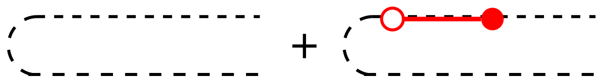
$< n\ (t)\ > =$

Keldysh Diagrammatic Monte Carlo

- Monte Carlo Sampling of Keldysh Perturbation Theory in $\color{red}{H_{tun}}$

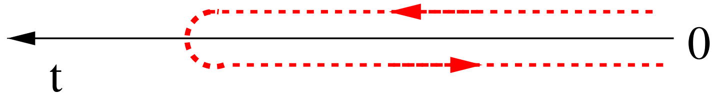


$$\langle O(t)\rangle = Tr\,\rho_0\,T_K\left(e^{i\int_K d\tau\, H_0+\color{red}{H_{tun}}}\,O\right)$$

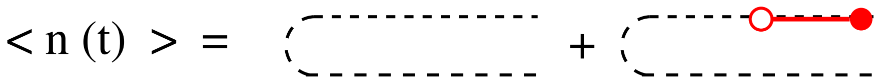
< n (t) > = 

Keldysh Diagrammatic Monte Carlo

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

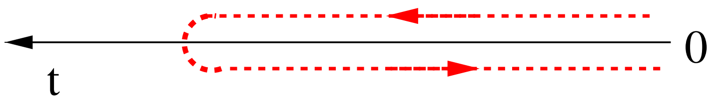


$$\langle O(t) \rangle = Tr\, \rho_0\, T_K \left(e^{i \int_K d\tau\, H_0 + H_{tun}}\, O \right)$$

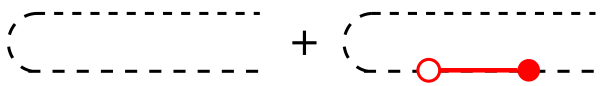


Keldysh Diagrammatic Monte Carlo

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

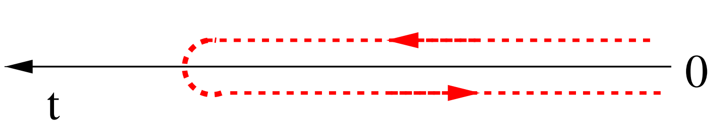


$$\langle O(t)\rangle = Tr\,\rho_0\,T_K\left(e^{i\int_K d\tau\, H_0+H_{tun}}\,O\right)$$

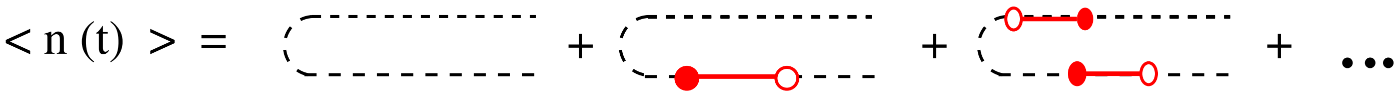
$\langle n(t) \rangle =$ 

Keldysh Diagrammatic Monte Carlo

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

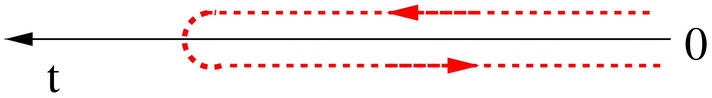


$$\langle O(t)\rangle = Tr\,\rho_0\,T_K\left(e^{i\int_K d\tau\, H_0+H_{tun}}\,O\right)$$

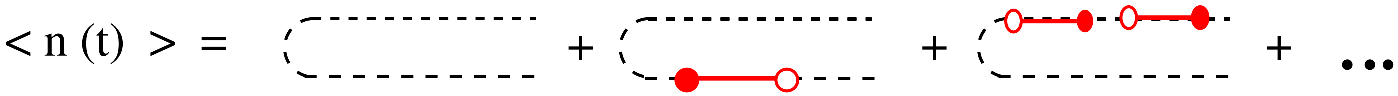


Keldysh Diagrammatic Monte Carlo

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

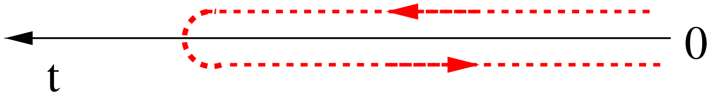


$$\langle O(t)\rangle = Tr\,\rho_0\,T_K\left(e^{i\int_K d\tau\, H_0+H_{tun}}\,O\right)$$

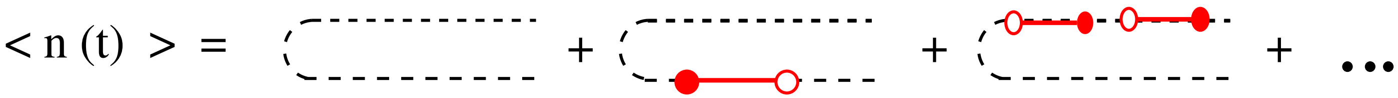


Keldysh Diagrammatic Monte Carlo

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



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

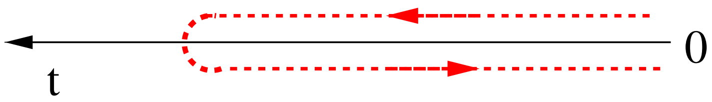


$$\langle\, n(t)\,\rangle = \sum_{n=0}^{\infty} \int det\Delta_{leads}(t_1^e, \cdots, t_n^e | t_1^s, \cdots t_n^s)\langle T_K \left\{ c(t_1^e)c^\dagger(t_1^s)\cdots c(t_n^e)c^\dagger(t_n^s) n(t) \right\}\rangle_{loc}$$

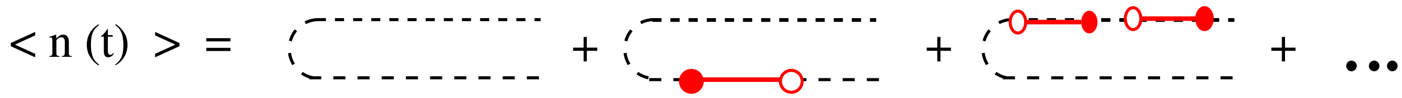
- Basic MC Updates: Adding/Removing/Shifting segments on the contour

Keldysh Diagrammatic Monte Carlo

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



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



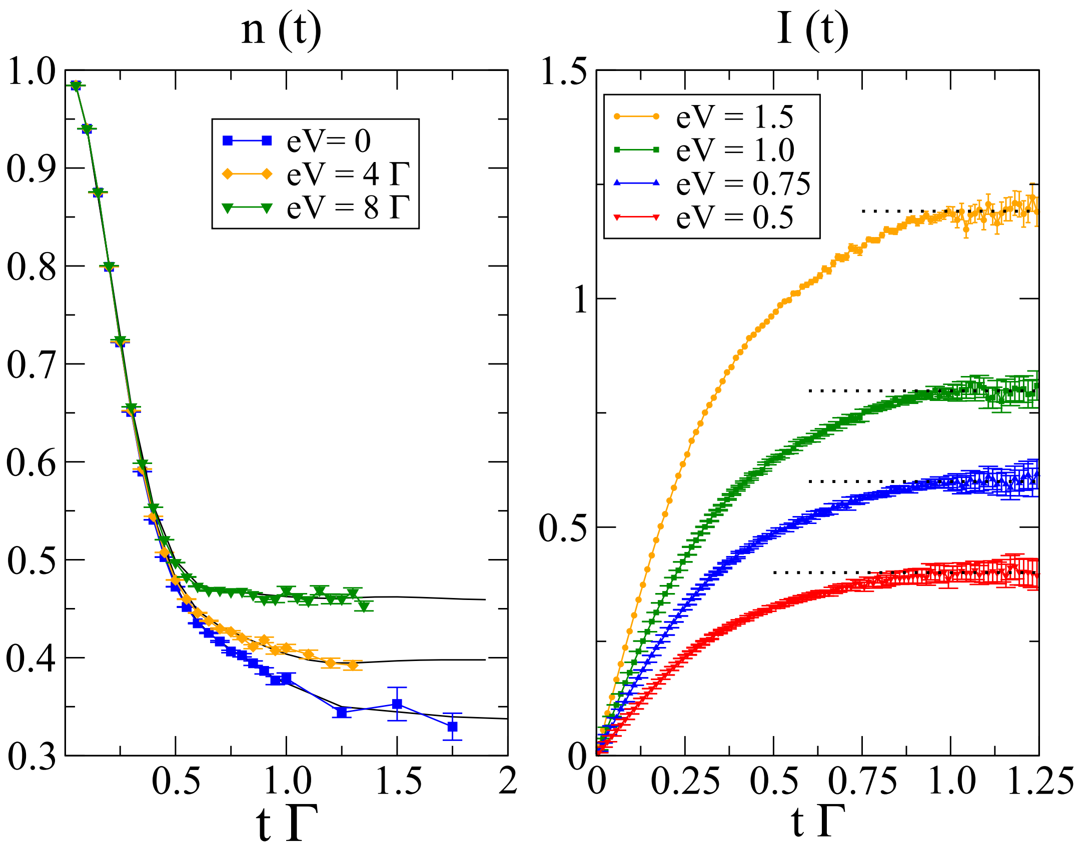
$$\langle n(t)\rangle = \sum_{n=0}^{\infty} \int det\Delta_{leads}(t_1^e, \cdots, t_n^e | t_1^s, \cdots t_n^s) \langle T_K \left\{ c(t_1^e) c^\dagger(t_1^s) \cdots c(t_n^e) c^\dagger(t_n^s) n(t) \right\} \rangle_{loc}$$

- 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!

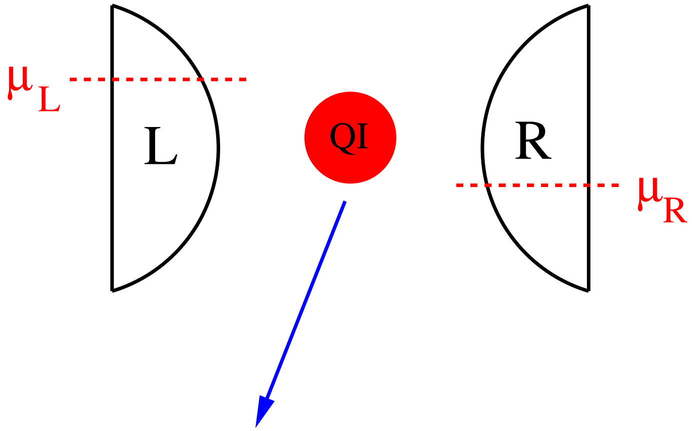
Benchmark: Biased Resonant Level Model



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

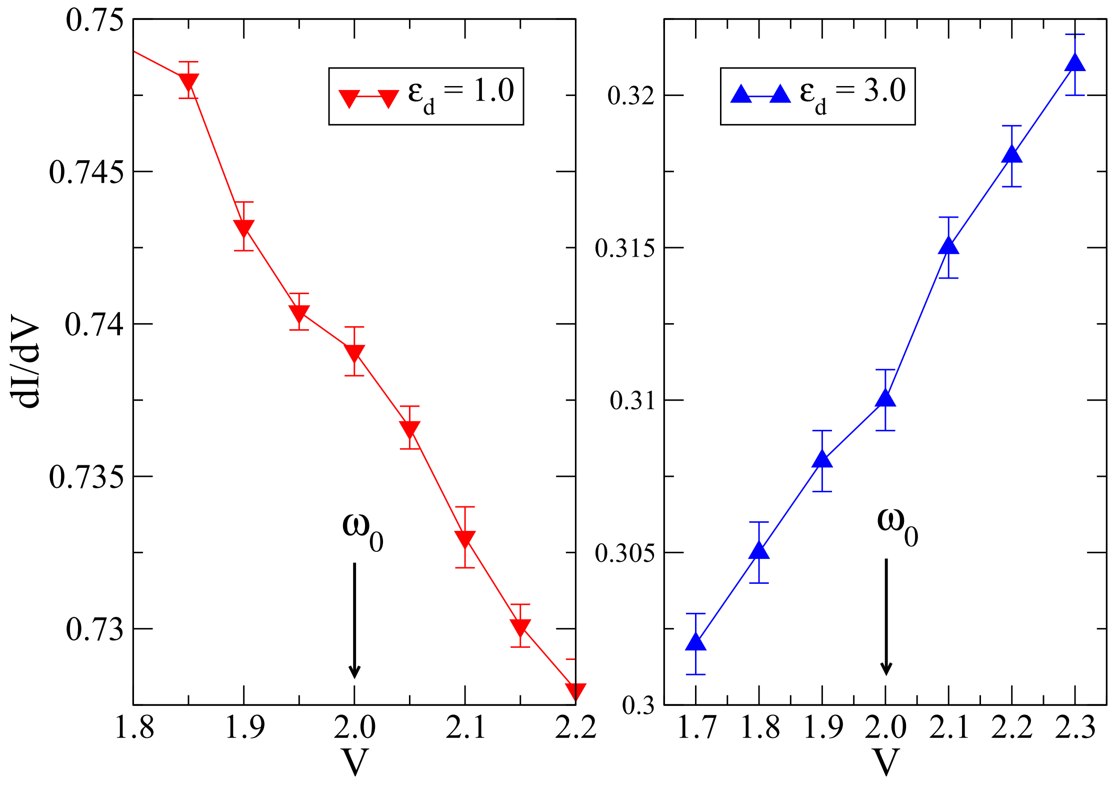
Non-Equilibrium Transport through a single molecule



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

- 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 $\longmapsto$ Current, Conductance
- No finite-size effects in the bath or in the dynamics
- Case Study: Inelastic Tunneling Spectra for a single-molecule conductor