Quantum transport through nano-devices
A scattering-states numerical renormalization group approach to open quantum

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Outline

1. Current through a nano-device
   • Kondo effect in single-electron transistors (SET)
   • finite bias transport: theoretical concepts

2. Theory of quantum transport
   • open quantum systems
   • scattering state NRG

3. Results
   • benchmark of the NEQ Green function algorithm
   • steady state spectra
   • comparison with Keldysh approaches
   • differential conductance in a magnetic field

4. Conclusion
   • open questions and problems
   • summary
1. Current through a nano-device
Molecular electronics - the future of computing
Molecular electronics - the future of computing

understanding of current transport:
electronics of the future
understanding of current transport: electronics of the future

emphasize: FUTURE

We still have to learn a lot
nano-scale device:

- **switching**: non-linear IV curves
- **physics interaction driven**
nano-scale device:

- switching: non-linear IV curves
- physics interaction driven

→ beyond the single-particle picture
Single electron transistor (SET)


weak coupling

on resonance

off resonance


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Single electron transistor (SET)


weak coupling

Kastner, RMP 64, 849(1992)
Single electron transistor (SET)

\[ E = \frac{e^2}{2C} \left( \hat{N} - N_g \right) \]


Kastner, RMP 64, 849(1992)
Single electron transistor (SET)


• eff. AF coupling: \[ H_I = J \vec{s}_b \vec{S}_{loc} \]

• Kondo effect: \[ T_K = D e^{-1/\rho J} \]

Single electron transistor (SET)


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Theoretical concepts

\[ \frac{e^2}{C} \]

\[ \mu_L \quad \mu_R \]

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Theoretical concepts

- lead and molecule/device separate entities
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hypothetically: lead and device initially disconnected, leads initially thermalized

• nano-device: a finite set of level
Theoretical concepts

- lead and molecule/device separate entities
  - hypothetically: lead and device initially disconnected, leads initially thermalized
- nano-device: a finite set of level
  - quantum-impurity problem
- leading order: sequential tunneling
Theoretical concepts

- rate equations

\[ e^2 \]

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Theoretical concepts

- rate equations
- Keldysh based approaches: perturbation theory (Caroli et al 1971), RG methods: Meir, Wingreen, Ueda, Oguri, Rosch, Wölfe, Kroha, Flensberg, Paaske, Thygesen, Millis, ...
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- scattering-states approaches: Hershfield, Metha, Andrei, Han, Oguri, FBA (2008)
Open quantum systems: finite size representation


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Open quantum systems: finite size representation

TD-DMRG Problems:

★ boundary condition: closed quantum system
Open quantum systems: finite size representation

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★ boundary condition: closed quantum system
★ Kondo problem: transient time $\propto 1/T_K$

TD-DMRG calculation: Schneider, Schmitteckert, arXiv:0601389
Open quantum systems: finite size representation

TD-DMRG Problems:
- ★ boundary condition: closed quantum system
- ★ Kondo problem: transient time $\propto 1/T_K$

How do we simulate an open system with a finite chain?
2. Theory of quantum transport

A scattering states approach
Boundary condition

Problem: steady state limit

- transient currents: \( \lim_{L \to \infty} \lim_{t \to \infty} J(t) = 0 \)
Boundary condition

Problem: steady state limit

- transient currents: \( \lim_{L \to \infty} \lim_{t \to \infty} J(t) = 0 \)
- steady state currents: \( J_{\infty} = \lim_{t \to \infty} \lim_{L \to \infty} J(t) > 0 \)
the challenge

• description of steady-state currents for arbitrary V, T, U, H
• using a finite size system
Open quantum systems

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• Coulomb interaction: Kondo effect, non-perturbative in equilibrium
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a solution


I. open quantum system: scattering states (Hershfield, Han, Oguri, Andrei)
Open quantum systems

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1. open quantum system: scattering states (Hershfield, Han, Oguri, Andrei)
2. density operator at finite bias but U=0 (Hershfield 1993)
   ⇒ NRG as solver at finite bias!
Open quantum systems

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- description of steady-state currents for arbitrary $V, T, U, H$
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1. open quantum system: scattering states (Hershfield, Han, Oguri, Andrei)
2. density operator at finite bias but $U=0$ (Hershfield 1993)  
   ⇒ NRG as solver at finite bias!
3. TD-NRG: evolve the system form $U=0$ to $U>0$ (Anders, Schiller 05, 06, 08)
\[ H = \sum_{k\sigma\alpha=L,R} \varepsilon_{k\sigma\alpha} c_{k\sigma\alpha}^\dagger c_{k\sigma\alpha} + \sum_{\sigma} E_{\sigma} d_{\sigma}^\dagger d_{\sigma} + U n_{\sigma}^d n_{\sigma}^d \]

\[ \sum_{k\sigma\alpha=L,R} t_{\alpha} \left( d_{\sigma}^\dagger c_{k\sigma\alpha} + c_{k\sigma\alpha}^\dagger d_{\sigma} \right) \]
1. Open quantum system: boundary condition

left and right-moving scattering states: $\gamma_{\epsilon\alpha\sigma}$
1. Open quantum system: boundary condition

- Left and right-moving scattering states: $\gamma_{\epsilon\alpha\sigma}$

- Itinerant states: device + L and R lead!
1. Open quantum system: boundary condition

- \( \gamma_{\varepsilon\alpha\sigma} \) left and right-moving scattering states:
- correct boundary condition
- complex: current carrying states

\( \gamma_{\varepsilon\alpha\sigma} \) itinerant states: device + L and R lead!
2. Open quantum system: scattering states

U=0: exact solution

- steady state density operator (Hershfield 93)

\[ \hat{\rho}_0(U = 0) = \frac{1}{Z_0} e^{-\beta(H_0 - \hat{Y}_0)} \]

\[ \hat{Y}_0 = \sum_{\alpha=L,R} \sum_{\sigma} \mu_{\alpha} \int d\epsilon \gamma^{\dagger}_{\epsilon \alpha \sigma} \gamma_{\epsilon \alpha \sigma} \]

- \( \gamma_{\epsilon \alpha \sigma} \) scattering states for itinerant L/R mover (Hershfield, Oguri)
2. Open quantum system: nano-device U=0

Wilson chain for right and left movers

\[ (\bar{V} = \sqrt{V_L^2 + V_R^2}, \; r_\alpha = V_\alpha / \bar{V}) \]

\[ d_\sigma = \frac{1}{\bar{V}} \sum_\alpha V_\alpha d_{\sigma \alpha} \]

\[ d_{\sigma \alpha} = \bar{V} \int d\varepsilon \sqrt{\rho(\varepsilon)} |G_0^{d}(\varepsilon + i\delta)|e^{i\Phi_0(\varepsilon)} \gamma_{\varepsilon \alpha \sigma} \]
2. Open quantum system: nano-device $U=0$

Wilson chain for right and left movers

- local d orbital

\[
\begin{align*}
\bar{V} &= \sqrt{V_L^2 + V_R^2}, \quad r_\alpha = \frac{V_\alpha}{\bar{V}} \\

\sigma d &= \frac{1}{\bar{V}} \sum_\alpha V_\alpha d_\sigma \alpha \\

\sigma d_\alpha &= \bar{V} \int d\varepsilon \sqrt{\rho(\varepsilon)} |G^{d}_0(\varepsilon + i\delta)| e^{i\Phi_0(\varepsilon)} \gamma_{\varepsilon \alpha \sigma}
\end{align*}
\]
2. Open quantum system: nano-device U=0

Wilson chain for right and left movers

- **local d orbital**
  \[
  \tilde{V} = \sqrt{V_L^2 + V_R^2}, \quad r_\alpha = V_\alpha / \tilde{V}
  \]

  \[
  d_\sigma = \frac{1}{\tilde{V}} \sum_\alpha V_\alpha d_{\sigma\alpha}
  \]

  \[
  d_{\sigma\alpha} = \tilde{V} \int d\varepsilon \sqrt{\rho(\varepsilon)} |G_0^{d}(\varepsilon + i\delta)| e^{i\Phi_0(\varepsilon)} \gamma_{\varepsilon\alpha\sigma}
  \]

- **novel NRG: discretisation of scattering states**
2. Open quantum system: nano-device U=0

price: current operator energy dependent

\[ I(\mu_L, \mu_R) = \frac{G_0}{e} \sum_{\sigma} \int \frac{d\varepsilon}{\pi} \left[ f_L(\varepsilon) - f_R(\varepsilon) \right] \text{Im} G_{0\sigma}^d(\varepsilon - i\delta) \]

\[ G_{0\sigma}^d(z) = r_R^2 \ll d_{\sigma R} |d_{\sigma R}^{\dagger} \rangle \langle z | + r_L^2 \ll d_{\sigma L} |d_{\sigma L}^{\dagger} \rangle \langle z | \]
3. Open quantum system: nano-device $U > 0$

left mover $\mu_l$

right mover $\mu_r$

fictitious junction

scattering states NRG

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3. Open quantum system: nano-device $U > 0$

- left mover $\mu_l$
- fictitious junction $U$
- right mover $\mu_r$

scattering states NRG

- switch on $H_U = Un^d_\uparrow n^d_\downarrow$: backscattering

$$d^\dagger_\sigma d_\sigma = \underbrace{r^2_R n^d_R}_{\text{density part}} + \underbrace{r^2_L n^d_L}_{\text{density part}} + r_R r_L \left( d^\dagger_{L\sigma} d_{R\sigma} + d^\dagger_{R\sigma} d_{L\sigma} \right)$$
3. Open quantum system: nano-device \( U > 0 \)

- switch on \( H_U = U n^d_{\uparrow} n^d_{\downarrow} \): backscattering

\[
d_{\sigma}^\dagger d_{\sigma} = r_R^2 n_{R\sigma}^d + r_L^2 n_{L\sigma}^d + r_R r_L \left( d_{L\sigma}^\dagger d_{R\sigma} + d_{R\sigma}^\dagger d_{L\sigma} \right)
\]

- absorb density term \( H_U^0 = \sum_{\alpha\alpha'} r_{\alpha}^2 r_{\alpha'}^2 n_{\alpha\uparrow} n_{\alpha\downarrow} \) in \( \rho_0 \rightarrow \tilde{\rho}_0 \)

scattering states NRG
3. Open quantum system: nano-device $U>0$

- **Left mover** $\mu_l$
- **Right mover** $\mu_r$
- **Fictitious junction** $U$

---

**scattering states NRG**

- **Switch on** $H_U = Un^{d\uparrow}_n n^{d\downarrow}_n$ : backscattering

\[
d^{\dagger}_{\sigma}d_{\sigma} = r^2_R n^{d}_{R\sigma} + r^2_L n^{d}_{L\sigma} + r_Rr_L \left( d^{\dagger}_{L\sigma}d_{R\sigma} + d^{\dagger}_{R\sigma}d_{L\sigma} \right)
\]

- **Density part**

- **Backscattering**

- **Absorb density term** $H^0_U = \sum_{\alpha\alpha'} r^2_{\alpha}r^2_{\alpha'} n_{\alpha\uparrow} n_{\alpha\downarrow}$ in $\rho_0 \rightarrow \tilde{\rho}_0$

- **Exact in the tunnel regime**
3. Open quantum system: nano-device $U>0$

\[
\hat{\rho}_\infty = \lim_{T \to \infty} \frac{1}{T} \int_0^T d\tau e^{-iH^f \tau} \tilde{\rho}_0 e^{iH^f \tau}
\]
3. Open quantum system: nano-device \( U > 0 \)

- left mover \( \mu_l \)
- fictitious junction
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scattering states NRG

- using the TD-NRG (FBA, Schiller 2005, 2006)

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- calculate finite $U$ non-equilibrium Green function
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$$\hat{\rho}_\infty = \lim_{T \to \infty} \frac{1}{T} \int_0^T d\tau e^{-iH_f \tau} \tilde{\rho}_0 e^{iH_f \tau}$$

steady state density operator

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1. scattering-state basis: boundary condition of an open quantum system
Summary of the scattering states NRG

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5. calculate NEQ spectral functions
   
Spin decay in the spin boson model close to the QCP
Time-dependent NRG

Spin decay in the AF Kondo model
Time-dependent NRG

Spin decay in the AF Kondo model

TD-NRG: Time scales of $10^8/D$ accessible!
3. Results
Benchmark: evolution from $U=0$ to finite $U$


symmetric single lead SIAM in equilibrium
Compare with Keldysh conserving approx.

conserving approximation
Compare with Keldysh conserving approx.
Compare with Keldysh conserving approx.
\( \frac{U}{\Gamma} = 8, \, R = \frac{\Gamma_L}{\Gamma_R} = 1, \, \mu_L = -\frac{V}{2}, \, \mu_R = \frac{V}{2} \)
Steady-state spectra: tunnel junction at finite bias

\[ U/\Gamma = 8, \quad R = \Gamma_L/\Gamma_R = 1000, \quad \mu_L = -r^2_R V, \quad \mu_R = r^2_L V \]
no magnetic field

\[ U/\Gamma = 8 \]
finite magnetic field \[ U/\Gamma = 8 \]
finite magnetic field \( U/\Gamma = 8 \)
Differential conductance

(d) $\beta=24$, $g_{ep}=0$

- $U=5$
- $U=5$, Anders ('08)
- $U=-5$

Comparision with Han, Heary
PRL 99, 2007,
Plot taken from Han, arxiv: 0906.5577
SNRG vs Hubbard I: local heating?

$T/\Gamma = 3.125, U = 20\Gamma$

- SNRG $V=0$
- Hubbard I $V=0$
- SNRG $V=4$
- Hubbard I $V=4$
- EQ-NRG $T/\Gamma = 3.9$


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4. Conclusion
Questions:
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- Kondo model: peak splitting?
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- limitation of the NEQ GF algorithm?
- Kondo model: peak splitting?
- calculation of the current directly?
- extension to more complex regions?
Summary

Scattering states NRG
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- novel approach to open quantum systems
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- novel approach to open quantum systems
- correct boundary condition
- include $U=0$ and the tunneling regime exactly
- TD-NRG used to evolve $\rho(\omega, U = 0) \rightarrow \rho(\omega, U > 0)$
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- first universal approach to all regimes of quantum transport
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Thank you for your attention!