Quantum Transport through Coulomb-Blockade Systems

Björn Kubala

Institut für Theoretische Physik III
Ruhr-Universität Bochum
Overview

• Motivation
  • Single-electron box/transistor
  • Coupled single-electron devices

• Model and Technique
  • Real-time diagrammatics

• Thermoelectric transport
  • Thermal and electrical conductance
  • Quantum fluctuation effects on thermopower

• Multi-island systems
  • Diagrammatics for complex systems
  • New tunneling processes
**Single-Electron Box**

Gate attracts charge to island.
Tunnel barrier $\rightarrow$ quantized charge

![Diagram of single-electron box](image)

Quantitatively:

$$E_{\text{ch}} = \frac{Q_L^2}{2C_J} + \frac{Q_R^2}{2C_g} + Q_R V_g$$

$$= \frac{e^2}{2C_{\Sigma}} (n - n_x)^2 + \text{const.},$$

Coulomb staircase
Single-Electron Transistor

Two contacts → transport

Quantitatively:

\[ E_{\text{ch}} = \frac{Q_L^2}{2C_J} + \frac{Q_R^2}{2C_g} + Q_R V_g \]

\[ = \frac{e^2}{2C_\Sigma} (n - n_x)^2 + \text{const.} \]
**Simple Coupled Device**

Box:

charge on $C_c$ (sawtooth)
input for transistor

Transistor:

Transistor measures box charge

one step of Coulomb staircase

(Lehnert et al. PRL ’03, Schäfer et al. Physica E ’03)
Overview

- **Motivation**
  - Single-electron box/transistor
  - Coupled single-electron devices

- **Model and Technique**
  - **Real-time diagrammatics**
  - Thermoelectric transport
    - Thermal and electrical conductance
    - Quantum fluctuation effects on thermopower
  - Multi-island systems
    - Diagrammatics for complex systems
    - New tunneling processes
Hamiltonian:  
\[ H = H_L + H_R + H_I + H_{\text{ch}} + H_T = H_0 + H_T \]

charge degrees of freedom separated from fermionic degrees:

charging energy

\[ H_{\text{ch}} = \frac{e^2}{2C}(\hat{N} - n_x)^2 \]

tunneling

\[ H_T = \sum_{r=R,L} \sum_{kln} (T_{rnl}^{kn} a_{kln}^{\dagger} c_{ln} e^{-i\varphi} + \text{h.c.}) \]

Time evolution of e.g. density matrix of charge governed by propagator \( \Pi \):

\[ \Pi_{n_1',n_1}^{n_2',n_2} = \text{Trace} \left[ \langle n_2'|\tilde{T} \exp \left(-i \int_{t_0}^{t} dt' H_T(t') I \right) |n_2 \rangle \langle n_1 | \exp \left(-i \int_{t_0}^{t} dt' H_T(t') I \right) |n_1' \rangle \right] \]

\( \Rightarrow \) Keldysh contour
Dyson-equation

Integrating out reservoirs/contracting tunnel vertices ⇒ each contraction ⇔ golden-rule rate:

\[
\alpha^r(\omega) = \int dE \alpha^r_0 f_r^\pm(E + \omega) f_r^\mp(E) = \pm \alpha^r_0 \frac{e^{\pm \beta (\omega - \mu_r)}}{1 - e^{\beta (\omega - \mu_r)}} \quad \text{with} \quad \alpha^r_0 = \frac{R_K}{4\pi^2 R_r}.
\]

Diagram with sequential, cotunneling and 3rd order processes

Write full propagator \( \Pi \) as Dyson equation:

\[
\Pi = \Pi^{(0)} + \Pi \Sigma \Pi^{(0)}
\]

with free propagator (w/o tunneling) \( \Pi^{(0)} \)

to calculate:

self-energy \( \Sigma \)
Overview

• Motivation
  • Single-electron box/transistor
  • Coupled single-electron devices

• Model and Technique
  • Real-time diagrammatics

• Thermoelectric transport
  • Thermal and electrical conductance
  • Quantum fluctuation effects on thermopower

• Multi-island systems
  • Diagrammatics for complex systems
  • New tunneling processes
Electrical and thermal conductance

\[ G_V = G_{as} \int d\omega \frac{\beta \omega/2}{\sinh \beta \omega} A(\omega) \quad ; \quad G_T = -G_{as} \frac{k_B}{e} \int d\omega \frac{(\beta \omega/2)^2}{\sinh \beta \omega} A(\omega) \]

\[ g_V = \frac{G_V}{G_{as}} \quad ; \quad g_T = -\frac{e}{k_B} \frac{G_T}{G_{as}} \]

perturbative expansion to 2nd order in coupling \( \alpha_0 \)

\[ g_{V/T} = g_{V/T}^{eq} + g_{V/T}^\alpha + g_{V/T}^\Delta + g_{V/T}^{\cot} \]

Thermoelectric transport:

\[ I = G_V V + G_T \delta T \]

\[ A(\omega) = [C^<(\omega) - C^>(\omega)] / (2\pi i) \]
Sequential tunneling

\[ g_{V/T} = g_{V/T}^{\text{seq}} + g_{V/T}^{\tilde{\alpha}} + g_{V/T}^{\tilde{\Delta}} + g_{V/T}^{\text{cot}} \]

- sequential tunneling:

\[ g_{V/T}^{\text{seq}} = \kappa_0 \frac{\beta \Delta_0/2}{\sinh \beta \Delta_0} \]

with \( \kappa_0 = \begin{cases} 1 & : \ V \\ \beta \Delta_0/2 & : \ T \end{cases} \)

Resonances around degeneracy points \( \Delta_n = 0 \).
Cotunneling

\[ g_{V/T} = g_{V/T}^{\text{seq}} + g_{V/T}^{\tilde{\alpha}} + g_{V/T}^{\tilde{\Delta}} + g_{V/T}^{\text{cot}} \]

- **standard cotunneling:**

\[
\begin{align*}
    g_{V}^{\text{cot}} &= \alpha_0 \frac{2\pi^2}{3} (k_B T)^2 \left( \frac{1}{\Delta_0} - \frac{1}{\Delta_{-1}} \right)^2 \\
    g_{T}^{\text{cot}} &= \alpha_0 \frac{8\pi^4}{15} (k_B T)^3 \left( \frac{1}{\Delta_0} - \frac{1}{\Delta_{-1}} \right)^2 \left( \frac{1}{\Delta_0} + \frac{1}{\Delta_{-1}} \right)
\end{align*}
\]

dominant away from resonance \(|\Delta_n| \gg k_B T|.

virtual occupation of unfavourable charged state.
Cotunneling

\[ g_{V/T} = g_{V/T}^{\text{seq}} + g_{V/T}^{\tilde{\alpha}} + g_{V/T}^{\tilde{\Delta}} + g_{V/T}^{\text{cot}} \]

\text{• standard cotunneling:}

\[ g_{V}^{\text{cot}} = \alpha_0 \frac{2\pi^2}{3} (k_B T)^2 \left( \frac{1}{\Delta_0} - \frac{1}{\Delta_{-1}} \right)^2 \]

\[ g_{T}^{\text{cot}} = \alpha_0 \frac{8\pi^4}{15} (k_B T)^3 \left( \frac{1}{\Delta_0} - \frac{1}{\Delta_{-1}} \right)^2 \left( \frac{1}{\Delta_0} + \frac{1}{\Delta_{-1}} \right) \]

\[ g_{V/T}^{\text{cot}} = \kappa_{-1} \Delta_{-1} \partial^2 \phi_{-1} + \kappa_0 \Delta_0 \partial^2 \phi_0 + \frac{\kappa_0 + \kappa_{-1}}{2} \frac{\phi_0 - \phi_{-1} + \Delta_{-1} \partial \phi_{-1} - \Delta_0 \partial \phi_0}{E_C} \]
Renormalized sequential tunneling

\[ g_{V/T} = g_{V/T}^{\text{seq}} + g_{V/T}^{\tilde{\alpha}} + g_{V/T}^{\tilde{\Delta}} + g_{V/T}^{\text{co}t} \]

- Renormalization of coupling:

\[ g_{V/T}^{\tilde{\alpha}} = \kappa_0 \frac{\beta \Delta_0 / 2}{\sinh \beta \Delta_0} \left[ \partial (2\phi_0 + \phi_{-1} + \phi_1) + \frac{\phi_{-1} - \phi_1}{E_C} \right] \]

- Energy gap:

\[ g_{V/T}^{\tilde{\Delta}} = \frac{\partial}{\partial \Delta_0} \left[ \kappa_0 \frac{\beta \Delta_0 / 2}{\sinh \beta \Delta_0} \right] (2\phi_0 - \phi_{-1} - \phi_1) \]

\[ \kappa_0 = \begin{cases} 1 & : V \\ \beta \Delta_0 / 2 & : T \end{cases} \]

Sequential tunneling but spectral density \( A(\omega) \) broadened and shifted.

\[ \downarrow \]

Renormalized parameters

- For coupling: \( \tilde{\alpha} \)
- Charging energy gap: \( \tilde{\Delta}_n \)
Renormalization by quantum fluctuations

\[
g_{V/T} = \kappa_0 \frac{\beta \Delta_0 / 2}{\sinh \beta \Delta_0} \left[ \partial \left( 2 \phi_0 + \phi_- + \phi_1 \right) + \frac{\phi_- - \phi_1}{E_C} \right]; \quad \tilde{g}_{V/T} = \frac{\partial}{\partial \Delta_0} \left[ \kappa_0 \frac{\beta \Delta_0 / 2}{\sinh \beta \Delta_0} \right] \left( 2 \phi_0 - \phi_- - \phi_1 \right)
\]

Quantum fluctuations \(\Rightarrow\) renormalization of system parameters

\[
G(\alpha_0, \Delta_0) = G_{\text{seq}}(\tilde{\alpha}, \tilde{\Delta}) + \cot. \text{ terms}
\]

expand:

\[
G_{\text{seq}}(\tilde{\alpha}, \tilde{\Delta}) = \tilde{\alpha} \frac{\partial G_{\text{seq}}(\alpha_0, \Delta_0)}{\partial \alpha_0} + \left( \tilde{\Delta} - \Delta_0 \right) \frac{\partial G_{\text{seq}}(\alpha_0, \Delta_0)}{\partial \Delta_0}
\]

renormalization of parameters (perturbative in \(\alpha_0\)):

\[
\begin{align*}
\tilde{\alpha} / \alpha_0 &= 1 - 2\alpha_0 \left\{ -1 + \ln \left( \frac{\beta E_C}{\pi} \right) - \partial \Delta_0 \left[ \Delta_0 \text{ Re } \Psi \left( i \frac{\beta \Delta_0}{2\pi} \right) \right] \right\} \\
\tilde{\Delta} / \Delta_0 &= 1 - 2\alpha_0 \left[ 1 + \ln \left( \frac{\beta E_C}{\pi} \right) - \text{ Re } \Psi \left( i \frac{\beta \Delta_0}{2\pi} \right) \right]
\end{align*}
\]

\(\tilde{\alpha}\) and \(\tilde{\Delta}\) decrease logarithmically by renormalization!

(for lowering temperature and increasing coupling \(\alpha_0\)) \(\Leftrightarrow\) many-channel Kondo-physics
Renormalization effects on $G_{V/T}$

$G(\alpha_0, \Delta_0) = G^{\text{seq}}(\tilde{\alpha}, \tilde{\Delta}) + \cot$ terms

$\tilde{\alpha}$ and $\tilde{\Delta}$ decrease logarithmically by renormalization:

- $\tilde{\alpha} \downarrow \rightarrow$ peak structure reduced by quantum fluctuations.
- $\tilde{\Delta} \downarrow \rightarrow$ closer to resonance; peak broadened by quantum fluct.

(logarithmic reduction of maximum electrical conductance (König et al. PRL ’97) experimentally observed by Joyez et al. PRL ’97)
Thermopower

Thermoelectric transport:

\[ I = G_V V + G_T \delta T \]

Thermopower:

\[ S = - \lim_{\delta T \to 0} \left. \frac{V}{\delta T} \right|_{I=0} = \frac{G_T}{G_V} \]

S measures average energy:

\[ S = - \frac{\langle \varepsilon \rangle}{eT}. \]
Charging energy gaps determine $S$

$\Delta_n = E_{\text{ch}}(n+1) - E_{\text{ch}}(n) = E_C \left[1 + 2(n - n_x)\right]$

A) at resonance:
- peak in $G_V$
- $S \propto \langle \varepsilon \rangle = 0$
- $\varepsilon \gtrless E_F$ cancels

B) sequential
- $G_V$ decays off resonance
- $S \propto \langle \varepsilon \rangle \propto \Delta_0 \propto n_x$

C) $n_x = 0 \Leftrightarrow \Delta_{-1} = -\Delta_0$
- two levels add for $G_V$
- two levels cancel for $S$
Sequential and cotunneling only

$S_{\text{seq+cot}} = S(\beta \Delta_0)$

- $SeT = \langle \varepsilon \rangle = \frac{g_V^{\text{seq}} \Delta_0/2 + g_V^{\text{cot}} (k_B T)^2 / \Delta_0}{g_V^{\text{seq}} + g_V^{\text{cot}}}$
- $S^{\text{seq}} = -\Delta_0/(2eT) \propto n_x \rightarrow \text{sawtooth}$
- sawtooth suppressed by cotunneling

\[ S^{\text{cot}} = -\frac{k_B}{e} \frac{4\pi^2}{5} \frac{1}{\beta \Delta_0} \]

How do quantum fluctuations change this picture?
Renormalization effects on thermopower

Low T properties governed by renormalization:

- Maximum of $S$

\[ S / (k_B/e) \]

- Charging-energy gap

\[ \langle \varepsilon \rangle / \Delta_0 \]

\(-S e T = \langle \varepsilon \rangle = \frac{g_V^{\text{seq}} \Delta_0 / 2 + g_V^{\text{cot}} (k_B T)^2 / \Delta_0}{g_V^{\text{seq}} + g_V^{\text{cot}}} \]

Crossover from $g_V^{\text{seq}}$ to $g_V^{\text{cot}} \Rightarrow$ maximum position

System closer to resonance $\Rightarrow$ crossover for larger $\Delta_{\text{max}}$

\[ \Rightarrow \text{Further support for renormalization picture!} \]

Reduced charging-energy gap

$\Rightarrow$ smaller $\langle \varepsilon \rangle$ (measures $\tilde{\Delta}$)
Overview

- Motivation
  - Single-electron box/transistor
  - Coupled single-electron devices

- Model and Technique
  - Real-time diagrammatics

- Thermoelectric transport
  - Thermal and electrical conductance
  - Quantum fluctuation effects on thermopower

- Multi-island systems
  - Diagrammatics for complex systems
  - New tunneling processes
Multi-island geometries:

parallel setup:  

series setup:  

Trivial changes allow application to different setups!  
(no changes in calculation of diagrams)
Algorithm for multi-island systems

E.g. parallel setup:

- **charge states**: \((t, b) \quad (1, 0)\)
- **Electrostatics**: 
  \[
  E_{ch}(t, b) = E_t(t - t_x)^2 + E_b(b - b_x)^2 + E_{coupl.}(t - t_x)(b - b_x)
  \]

- **generate all diagrams**:
  - start from any charge state
  - choose vertex positions
  - choose tunnel junctions and directions of lines
  - connect vertices
  - change charge states

- **Calculate value of diagram**, contributing to
  \[
  \sum(t,b) \rightarrow (t,b-1)
  \]

Simple rules but plenty of diagrams (in 2nd order \(2^{11}\) per charge state)

\[\Rightarrow\] Automatically generate and calculate all diagrams!
New processes in coupled SETs

-before:
  - study building blocks separately
  - link blocks together:
    e.g., average charge of one SET → input for other SET

-full treatment:
  - complete 2nd order theory
  - quantum fluctuations
  - backaction of SET on box
  - new class of processes:
    double-island cotunneling with energy exchange
    ⇒ noise ↔ $P(E)$ theory
    (SET1 noisy environment for SET2)
Noise assisted tunneling

limiting cases:
- **small** driving
detector-cotunneling independent of $I_g$

- **strong** driving of generator
$$P(E) \propto \frac{S_g^Q}{E^2} \leftarrow \text{generator noise}$$
$$\Gamma_{01}^d = \Gamma(\Delta^d) = \alpha_0 \int dE \frac{E}{1 - e^{-\beta E}} P(-\Delta^d - E)$$

noise-assisted tunneling $\propto |I_g|$ 
(instead of exponential suppression).

\[ P(n_g = 0) \approx \frac{1}{2} \approx P(n_g = 1) \]
\[ P(n_d = 0) \approx 1 \]
\[ P(n_d = 1) \neq 0 \]
by noise-assisted tunneling

![Graphs showing I$_D$ vs. $V_G^{sd}/2$ for different $V_G^{sd}/2$ values]
Conclusions

- Higher-order tunneling effects beside cotunneling
- Thermoelectric properties of an SET
  - Quantum fluctuations renormalize system parameters
  - Electrical and thermal conductance renormalized similarly
  - Thermopower measures average energy ⇒ logarithmic (Kondo-like) reduction of charging-energy gap
- General scheme to analyze multi-island systems
  - All 2nd order diagrams computed automatically
  - Detailed study of mutual influence of coupled SETs possible, backaction and quantum fluctuations
  - New tunneling processes exchange energy between islands