Quantum thermodynamics: transport in strongly coupled systems

Caio Lewenkopf
Universidade Federal Fluminense

Instituto de Física
Universidade Federal Fluminense

Anton Bruch

Felix von Oppen

Anton Bruch, CL, and Felix von Open
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Outline

1. **Entropy production in electronic transport (status)**

   weak and strong coupling

   system-bath partition

2. **Minimum model**

3. **Landauer-Büttiker approach**

   charge and energy currents

   stationary limit: heat and entropy currents

   entropy evolution under a time-dependent drive

Entropy production: Boltzmann H-theorem

collision integral: route to equilibrium

$$\left(\frac{\partial f(p_1)}{\partial t}\right)_{\text{col}} = \int dp_2 dp_1' dp_2' \delta(P_f - P_i)|T_{\text{fi}}|^2(f_2' f_1' - f_2 f_1)$$

$$S(t) \equiv -H(t) = \int d\mathbf{p}\, f(\mathbf{p},t) \ln f(\mathbf{p},t)$$

Boltzmann

H-theorem (1873)

$$\frac{dH(t)}{dt} \leq 0$$

$$\frac{dS(t)}{dt} \geq 0$$

equilibrium $\frac{dH(t)}{dt} = 0$ implies that $f(\mathbf{p},t) \to f_0(\mathbf{p})$

Maxwell-Boltzmann

Entropy production: Quantum kinetic approach

e.g., Kita, Prog. Theor. Phys. (2010)

quasi-static, close-to-equilibrium limit - Wigner transformation

NEGF
Green's functions

$$G^{<}(\mathbf{p}E;\mathbf{r}t) = iA(\mathbf{p}E;\mathbf{r}t)\phi(\mathbf{p}E;\mathbf{r}t)$$

"local"
entropy
density

$$\sigma[\phi] = -\phi\log\phi - (1-\phi)\log(1-\phi)$$

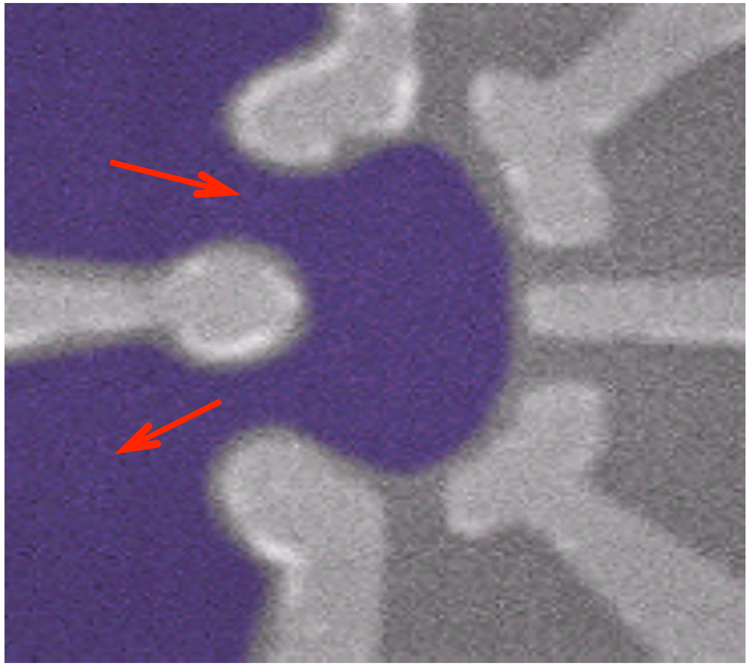
$$\phi \equiv \phi(\mathbf{p}E;\mathbf{r}t)$$

continuity
equation

$$\frac{\partial s}{\partial t} + \nabla\cdot\mathbf{j}_s = \frac{\partial s_{\mathrm{coll}}}{\partial t}$$

Mesoscopic electronic transport

billiard-like "idealization"



L

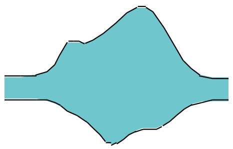
quantum dot

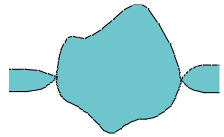
quantum regime

$$\ell_\phi \gg L$$

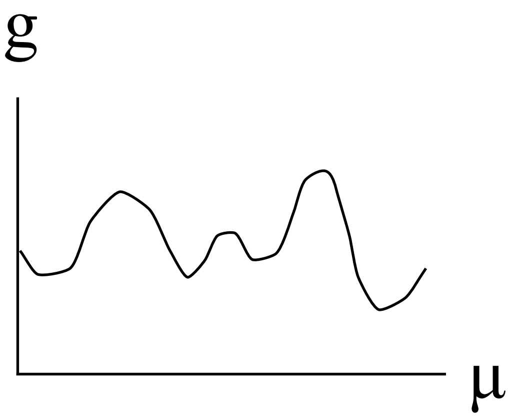
ℓ_ϕ quantum coherence length

From open to isolated





WIDE OPEN



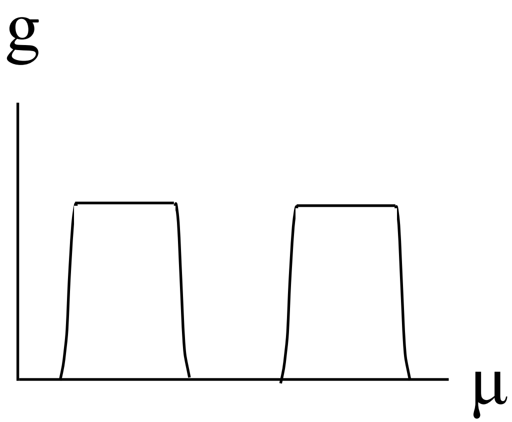
Strong coupling:

Charged fluid without blockade in the conduction

$$\Gamma >> \Delta$$

e-e interactions "unimportant"

INTENSE TUNNELING



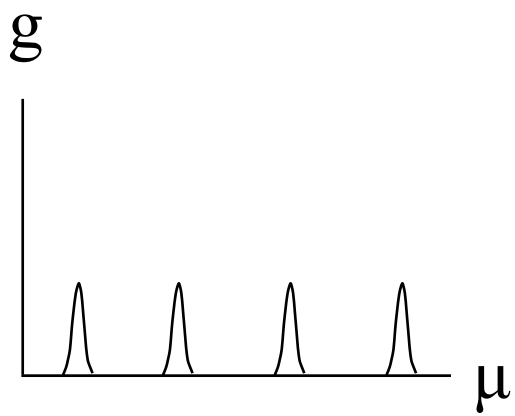
Intermediate coupling:

h/(RC)~U. charging energy starts affecting transport

$$\Gamma \sim \Delta$$

$$T \leq T_K$$

WEAK TUNNELING

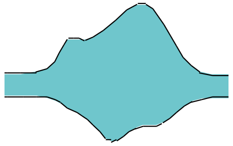


Weak coupling:

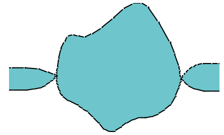
Discrete charge tunneling strong Coulomb blockade

$$\Gamma << \Delta$$

$$\Gamma << T$$



From open to isolated



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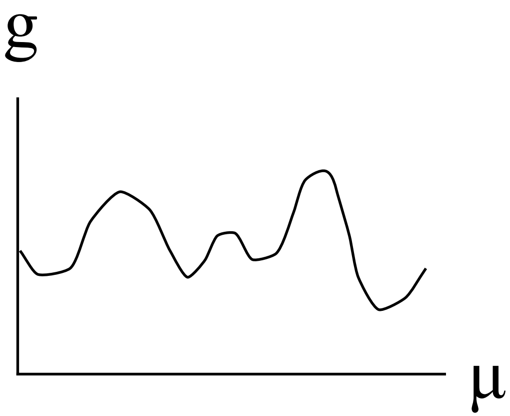
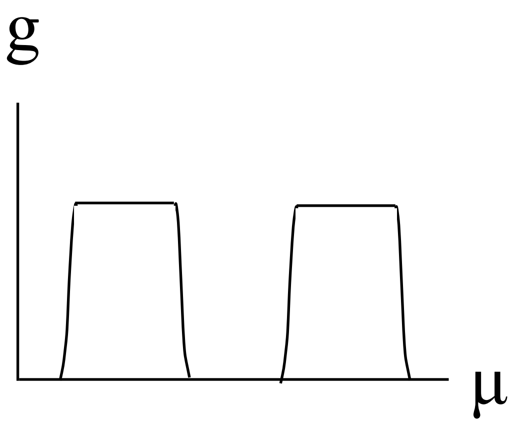
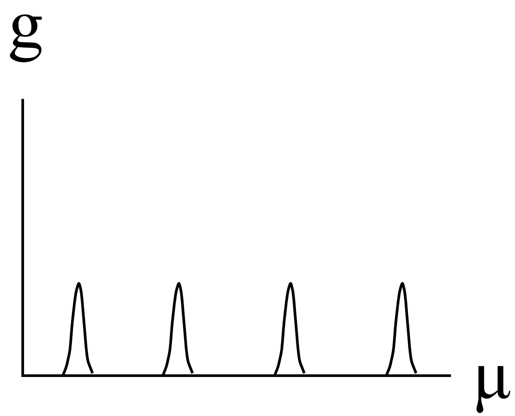


INTENSE TUNNELING



WEAK TUNNELING



coupling

Open dots
bilinear
Hamiltonian

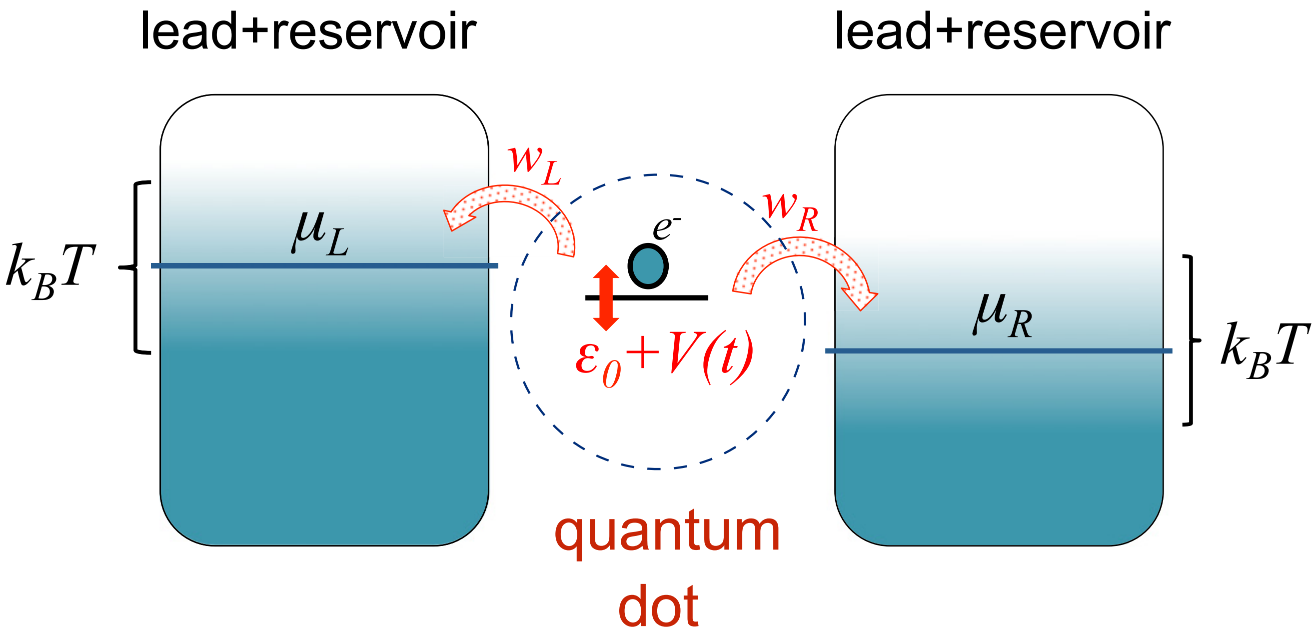
many-body
correlations

Kondo regime
non-perturbative
techniques

perturbative
expansion

Coulomb blockade
beyond mean field
rate equations

Strong coupling: the minimal model



$$H_{\mathrm{D}}(t) = \varepsilon_0(t) d^\dagger d$$

$$H = H_{\mathrm{D}}(t) + H_{\mathrm{V}} + H_{\mathrm{B}}$$

$$H_{\mathrm{V}} = \sum_{k\alpha} \left(W_\alpha d^\dagger c_{k\alpha} + \mathrm{H.c.} \right)$$

partition

$$H_{\mathrm{B}} = \sum_{k\alpha} \varepsilon_{k\alpha} c^\dagger_{k\alpha} c_{k\alpha}$$

NEGF solution

PRL **114,** 080602 (2015) PHYSICAL REVIEW LETTERS week ending 27 FEBRUARY 2015

Quantum Thermodynamics: A Nonequilibrium Green's Function Approach

M. Esposito, M. A. Ochoa, M. Galperin

spectral function

$$A(t,E) = \frac{\Gamma(t,E)}{[E - \varepsilon(t) - \Lambda(t,E)]^2 + [\Gamma(t,E)/2]^2}$$

renormalized spectral function

$$\mathcal{A}(t,E) = A(1 - \partial_E \Lambda) + \Gamma \partial_E \mathrm{Re} G^r$$

equilibrium

$$\sigma(E) = -f(E)\ln f(E) - [1 - f(E)]\ln[1 - f(E)]$$

$$G^<(E) = iA(E)f(E)$$

non-equilibrium
ansatz

$$\sigma(E,t) = -\phi(E,t)\ln\phi(E,t) - [1 - \phi(E,t)]\ln[1 - \phi(E,t)]$$

$$G^<(E,t) = i\mathcal{A}(E,t)\phi(E,t)$$

problems of the NEGF solution

$$N(t) = \int \frac{dE}{2\pi} \mathcal{A}(t,E)\phi(t,E)$$

$$\mathcal{E}(t) = \int \frac{dE}{2\pi} \mathcal{A}(t,E) E\, \phi(t,E)$$

$$S(t) = \int \frac{dE}{2\pi} \mathcal{A}(t,E)\sigma(t,E)$$

strong coupling?

$\mathcal{A}(t,E)$

(ad hoc) "system" spectral function

approach satisfies the laws of thermodynamics and describes irreversible driving

but

- "standard spectral function fails to obtain the second law”
- approach does not give the equilibrium forms of thermodynamic functions at the quasi-static limit

Improvement

A. Bruch, M. Thomas, S. Viola-Kusminskiy, F. von Oppen, A. Nitzan, PRB (2016)

Single-terminal quantum dot (minimal model)

(adiabatic) expansion in powers of the **driving velocity**

zero order
equilibrium

$$\Omega_{\text{tot}} = -k_B T \int \frac{d\varepsilon}{2\pi} \rho(\varepsilon) \ln(1 + e^{-\beta(\varepsilon-\mu)}),$$

$$E^{(0)} = \Omega + \mu N^{(0)} + T S^{(0)} = \int \frac{d\varepsilon}{2\pi} \varepsilon A f. \qquad dE^{(0)} = dW^{(0)} + dQ^{(0)} + \mu dN^{(0)}$$

first order
quasi-static
(reversible)

$$\dot{E}^{(1)} = \dot{\varepsilon}_d \frac{\partial E^{(0)}}{\partial \varepsilon_d} = \dot{\varepsilon}_d \int \frac{d\varepsilon}{2\pi} \varepsilon \frac{\partial A}{\partial \varepsilon_d} f$$

$$\dot{Q}^{(1)} = T \dot{\varepsilon}_d \frac{\partial S^{(0)}}{\partial \varepsilon_d} = \dot{\varepsilon}_d \int \frac{d\varepsilon}{2\pi} (\varepsilon - \mu) A \partial_\varepsilon f$$

second order
(irreversible)

$$\dot{W}^{(2)} = -\frac{\dot{\varepsilon}_d^2}{2} \int \frac{d\varepsilon}{2\pi} \partial_\varepsilon f A^2 \qquad \dot{Q}^{(2)} = -\frac{\dot{\varepsilon}_d^2}{2} \int \frac{d\varepsilon}{2\pi} (\varepsilon - \mu) \partial_\varepsilon^2 f A^2$$

Improvement: partition issue

strong coupling: symmetric splitting

quasi-static (reversible)
first order in drive

$$\dot{Q}^{(1)} = \dot{\varepsilon}_d \int \frac{d\varepsilon}{2\pi} (\varepsilon - \mu) A \partial_\varepsilon f$$

from thermodynamic relations

$$\dot{Q}^{(1)} = T \dot{\varepsilon}_d \frac{\partial S^{(0)}}{\partial \varepsilon_d}$$

from microscopic model

$$\dot{Q}^{(1)} = -\frac{d}{dt} \left\langle H_B + \frac{1}{2} H_V \right\rangle^{(0)} - \mu \frac{d}{dt} N^{(0)}$$

System-bath partition: transport vs. thermodynamics

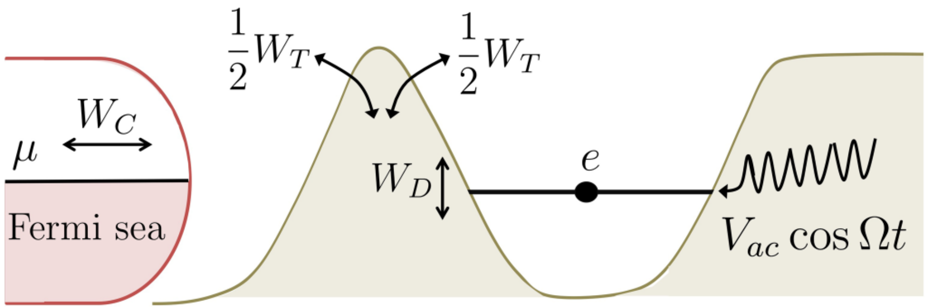
Odashima and CHL, PRB (2017)

Electronic transport:

partition and partition-free approaches give the same results for time-dependent transport (wide band limit)

Thermal transport:

symmetric splitting



Moskalets, Arrachea, Sánchez, PRB (2014)

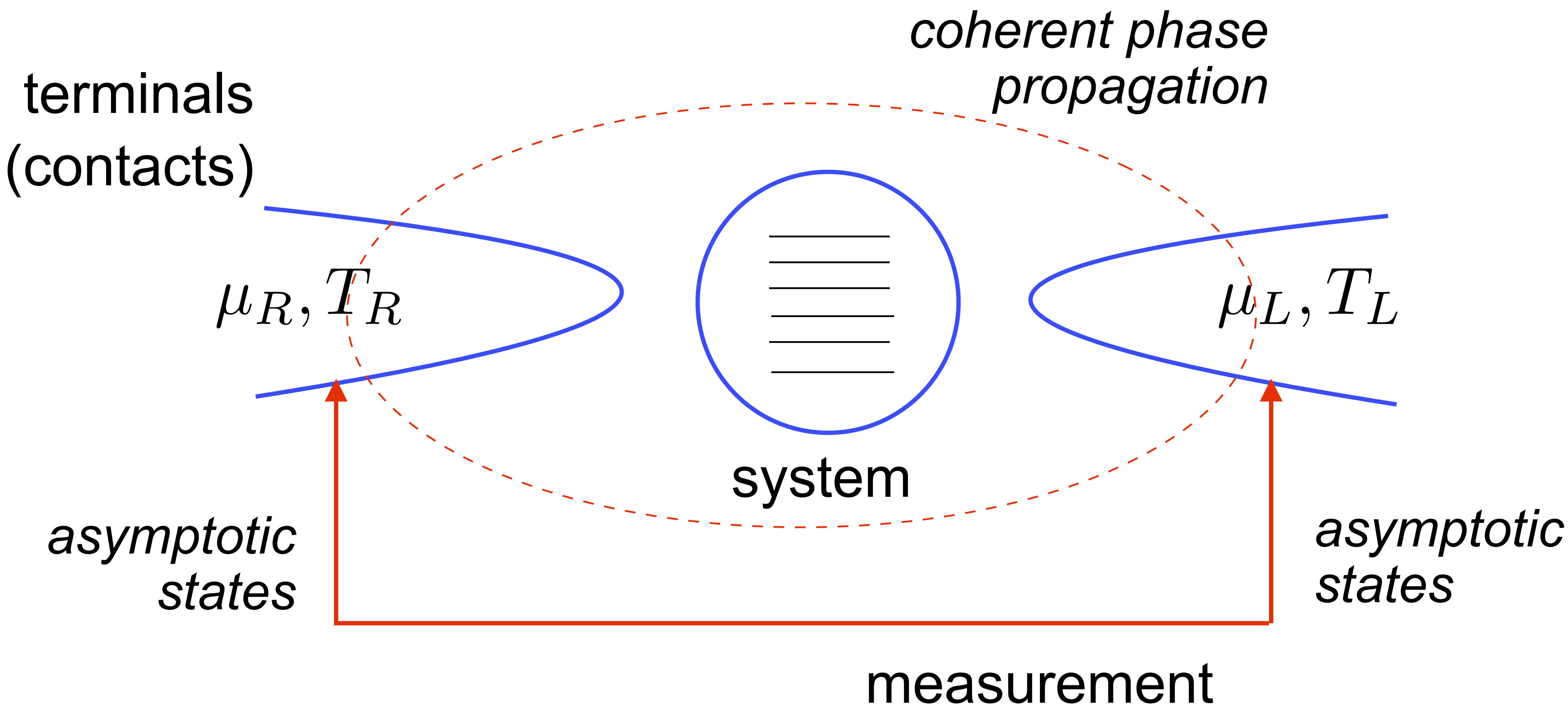
fluctuations?

Esposito, Ochoa, and Galperin, PRB (2015)

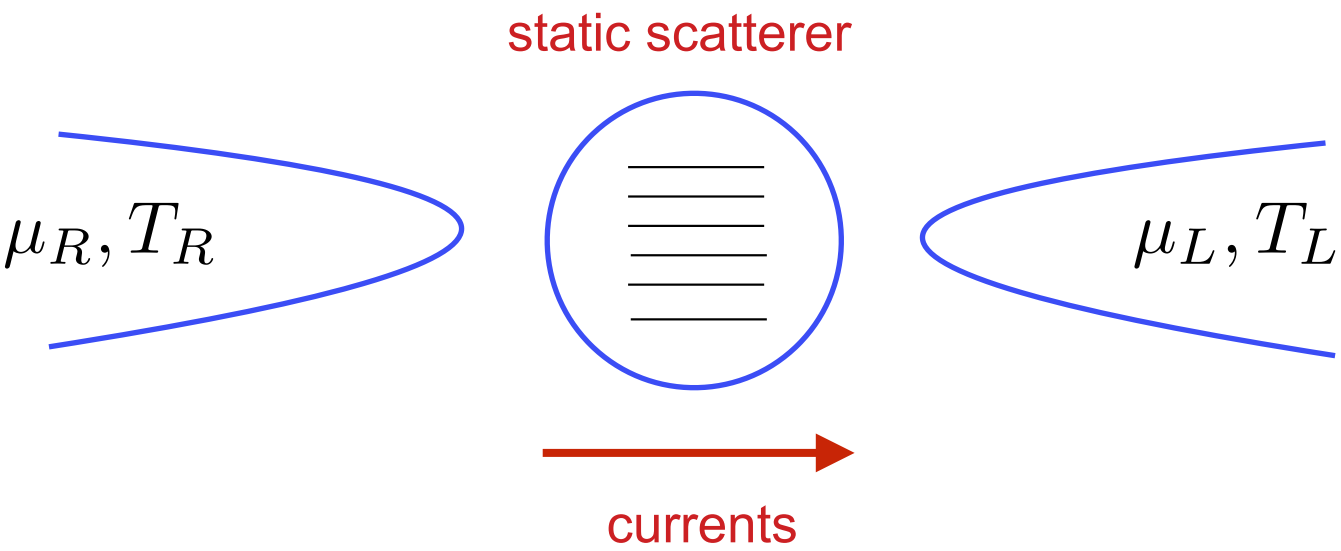
Ochoa, Nitzan, Bruch, PRB (2016)

Landauer-Büttiker approach

conductance is transmission!



Entropy production in "thermoelectrics"



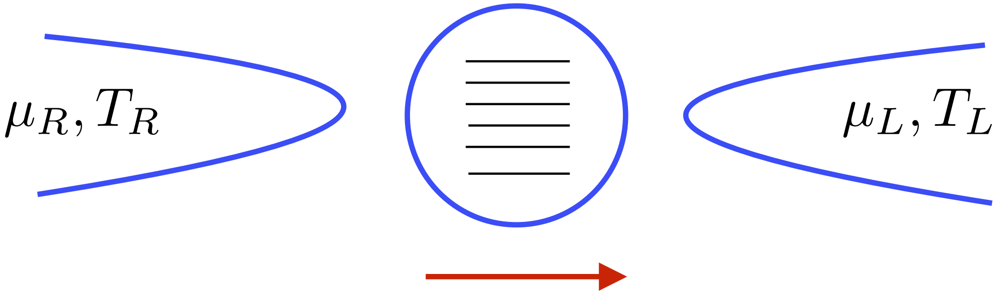
$$TdS = dE - \mu dN$$

$$\dot{S} = \frac{\dot{E}_L - \mu_L \dot{N}_L}{T_L} + \frac{\dot{E}_R - \mu_R \dot{N}_R}{T_R}$$

energy and particle conservation,
small temperature difference

$$\dot{S} = I_Q \frac{\Delta T}{T^2} + I_N \frac{\Delta \mu}{T}$$

Entropy production in "thermoelectrics"



linear response

$$\begin{pmatrix} I_N \\ I_Q \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$$

$$X_1 = \frac{\Delta\mu}{T}$$

$$X_2 = \frac{\Delta T}{T^2}$$

entropy production

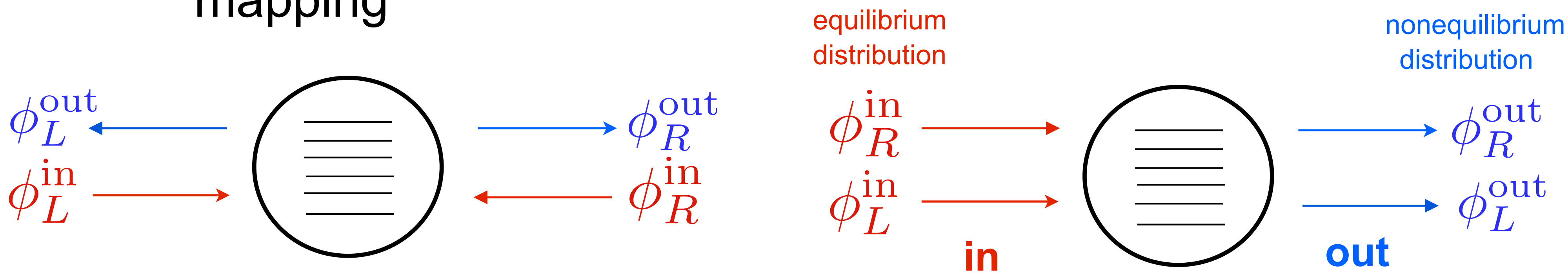
$$\dot{S} = (X_1, X_2)\,\mathbf{L} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$$

$$\Delta T = 0 \longrightarrow \dot{S} = L_{11} X_1^2 = \frac{1}{T} G V^2$$

Entropy production: microscopic construction

Mehta, Andrei, PRL (2008)

mapping



$$\dot{S} = \lim_{L\to\infty} \frac{1}{L} \sum_p \sum_{\alpha=L,R} v_F [\phi_\alpha^{\text{out}}(p) - \phi_\alpha^{\text{in}}(p)] \frac{\varepsilon_p - \mu_\alpha}{T}$$

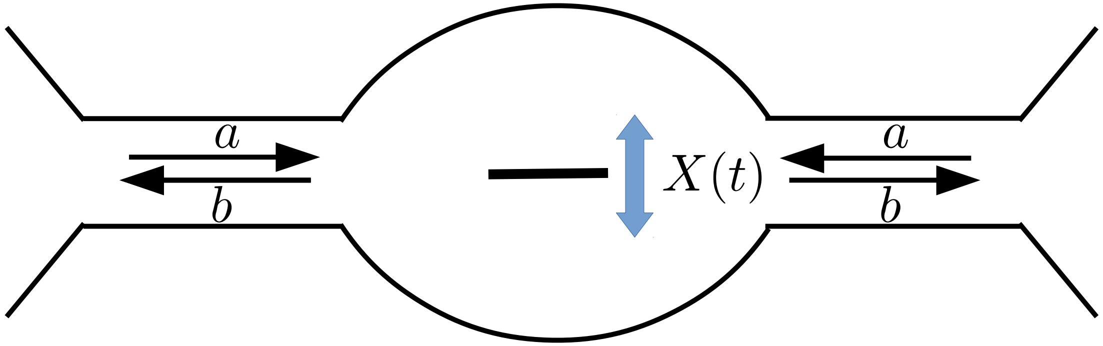
$$\dot{S} = \lim_{L\to\infty} \frac{1}{L} \sum_{\alpha=L,R} v_F \Big([\sigma(\phi_\alpha^{\text{out}}) - \sigma(\phi_\alpha^{\text{in}})] + D_{\text{KL}}[\phi_\alpha^{\text{out}} || \phi_\alpha^{\text{in}}] \Big)$$

Shannon entropy $\sigma(\phi) = -\sum_p (1-\phi(\epsilon_p)) \ln(1-\phi(\epsilon_p)) - \sum_p \phi(\epsilon_p) \ln \phi(\epsilon_p)$

relative (Kullback-Leibler) entropy $D_{\text{KL}}[P||Q] = -\sum_p P(\epsilon_p) \ln \frac{Q(\epsilon_p)}{P(\epsilon_p)}$

Scattering approach

A. Bruch, CHL, F. von Oppen, PRL (2018)



sketch of a quantum dot under an external drive

S-matrix:
$$\begin{pmatrix} b_1(\epsilon) \\ \vdots \\ b_N(\epsilon) \end{pmatrix} = \int \frac{d\epsilon'}{2\pi} \mathcal{S}(\epsilon, \epsilon') \begin{pmatrix} a_1(\epsilon') \\ \vdots \\ a_N(\epsilon') \end{pmatrix}$$

$$\langle a^\dagger_\beta(\epsilon) a_\alpha(\epsilon') \rangle = \phi^{\text{in}}_{\alpha\beta}(\epsilon) 2\pi \delta(\epsilon - \epsilon')$$

incoming states

$$\phi^{\text{in}}_{\alpha\beta}(\epsilon) = \delta_{\alpha\beta} f_\alpha(\epsilon)$$

Scattering approach

Wigner transform $$\phi^{\text{out}}_{\alpha\beta}(t,\epsilon) = \int \frac{d\tilde{\epsilon}}{2\pi} e^{-i\tilde{\epsilon}t} \left\langle b^{\dagger}_{\beta}(\epsilon - \tilde{\epsilon}/2) b_{\alpha}(\epsilon + \tilde{\epsilon}/2) \right\rangle$$

currents

particle $$I^N_\alpha(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \left\{ \phi^{\text{out}}_{\alpha\alpha}(t,\epsilon) - \phi^{\text{in}}_{\alpha\alpha}(\epsilon) \right\}$$

energy $$I^E_\alpha(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi}\, \epsilon \left\{ \phi^{\text{out}}_{\alpha\alpha}(t,\epsilon) - \phi^{\text{in}}_{\alpha\alpha}(\epsilon) \right\}$$

heat $$I^Q_\alpha(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} (\epsilon - \mu) \{ \phi^{\text{out}}_{\alpha\alpha}(t,\epsilon) - \phi^{\text{in}}_{\alpha\alpha}(\epsilon) \}$$

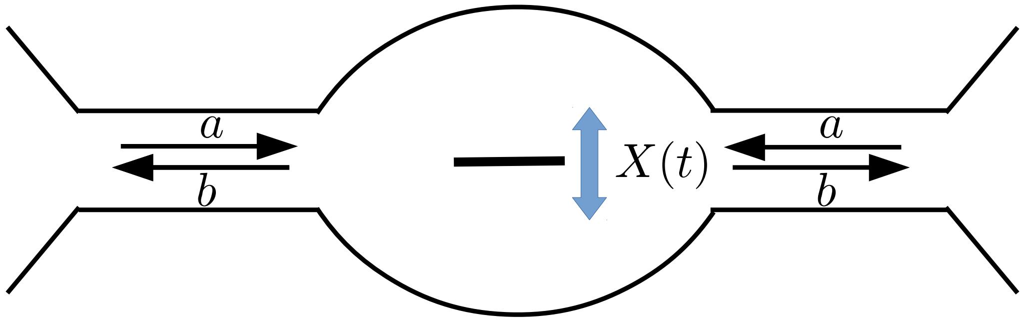
$$\varrho_\alpha(\epsilon) = [2\pi v_\alpha(\epsilon)]^{-1}$$

$$I^Q_\alpha = I^E_\alpha - \mu_\alpha I^N_\alpha$$

entropy density $$\sigma[f_\alpha(\epsilon)] = -f_\alpha(\epsilon) \ln f_\alpha(\epsilon) - (1 - f_\alpha(\epsilon)) \ln(1 - f_\alpha(\epsilon))$$

entropy current $$I^S_{\text{tot}}(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \operatorname{tr}_c \left\{ \sigma[\phi^{\text{out}}(t,\epsilon)] - \sigma[\phi^{\text{in}}(\epsilon)] \right\}$$

Dynamic scatterer



external drive (zero bias)

$$\varepsilon = \varepsilon_0 + V[X(t)] \qquad f_\alpha(\epsilon) = f(\epsilon)$$

expansion in powers of the drive

$$\mathcal{S}(\epsilon, t) = S_t(\epsilon) + \dot{X} A_t(\epsilon) + \dot{X}^2 B_t(\epsilon)$$

$$\phi^{\text{out}} \simeq \hat{I}\, f + \phi^{\text{out}(1)} + \phi^{\text{out}(2)}$$

collecting everything

$$\boxed{I^S_{\text{tot}} = \frac{I^Q_{\text{tot}}}{T} - \frac{\dot{W}^{(2)}}{T}}$$

$$\dot{W}^{(2)} = -\frac{\dot{X}^2}{2} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \partial_\epsilon f(\epsilon) \text{tr}_c \left(\partial_X S^\dagger \partial_X S \right) \geq 0$$

dissipated power pumped by the drive
back action force

Entropy evolution: inside-outside duality

$$\frac{ds}{dt} + I^S_{\text{tot}} = 0\,.$$

entropy stored in the QD
inside

entropy current
outside

source-free
von Neumann entropy

$$S(t) = -\text{tr}\rho(t)\ln\rho(t) = -\text{tr}\rho(0)\ln\rho(0) = S(0)$$

"inside" unitary evolution

averaged over a cycle $\quad I^S_{\text{tot}} = \frac{I^Q_{\text{tot}}}{T} - \frac{\dot{W}^{(2)}}{T}$

$$\overline{I^{Q(2)}_{\text{tot}}} = \overline{\dot{W}^{(2)}}$$

energy pumped by the drive
is released as heat

Conclusions

1. Landauer-Büttiker-like approach avoids partition problem and allows one to treat strongly coupled systems

2. The inside-outside duality recovers the expressions for entropy production obtained from standard thermoelectrics

3. The approach reproduces the expressions for single a lead in the wide band limit

4. The theory is consistent with the laws of thermodynamics and the quasi-static limit