Landauer-Büttiker approach to strongly coupled quantum thermodynamics: inside-outside duality of entropy evolution

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Collaborators

- **Inside approach**

  *Quantum thermodynamics of the driven resonant level model*


  w/ Anton Bruch, Mark Thomas, Silvia Kusminskiy & Abraham Nitzan

- **Outside approach**

  *Landauer-Büttiker approach to strongly coupled quantum thermodynamics: inside-outside duality of entropy evolution*


  w/ Anton Bruch & Caio Lewenkopf
Classic(al) heat engine

First law \[ dU = dW + dQ \]

Second law \[ \frac{dS}{dt} = \frac{\dot{Q}}{T} + \dot{S}_i \quad \dot{S}_i \geq 0 \]

max. efficiency \[ \eta_C = \frac{T_H - T_C}{T_H} \]
Nano-engine

**First law**
\[ dU = dW + dQ \]

**Second law**
\[ \frac{dS}{dt} = \frac{\dot{Q}}{T} + \dot{S}_i \quad \dot{S}_i \geq 0 \]
Quantum thermodynamics

- strong fluctuations
- quantum dynamics & quantum coherence
- quantum entanglement & quantum measurement
- strong system-bath coupling (unlike small surface-to-volume ratio for macroscopic systems)

system-bath coupling cannot be neglected
This talk

- strong fluctuations
- quantum dynamics & quantum coherence
- quantum entanglement & quantum measurement
- strong system-bath coupling (unlike small surface-to-volume ratio for macroscopic systems)

System-bath coupling cannot be neglected
Central result

Entropy production

\[ \dot{S}_i = \frac{\dot{X}^2}{2T} \int \frac{d\varepsilon}{2\pi} (-\partial_\varepsilon f) \text{tr}_c (\partial_X S^+ \partial_X S) \geq 0 \]

- arbitrary nanostructure with coherent quantum dynamics
- non-interacting electrons
- transparent physical interpretation
Driven resonant level model

Hamiltonian

\[ H = H_D + H_V + H_B \]

- **dot level**
  \[ H_D = \epsilon_d(t)d^\dagger d \]

- **leads**
  \[ H_B = \sum_k \epsilon_k c_k^\dagger c_k \]

- **dot-lead coupling**
  \[ H_V = \sum_k (V_k d^\dagger c_k + \text{H.c.}) \]

- non-interacting electrons
- adiabatic variation of \( \epsilon_d, V_k \) (slow compared to \( \Gamma \))
- non-equilibrium beyond quasi-static limit
Strong system-reservoir coupling

- full quantum coherence
- strong coupling: $\Gamma \gg T$ and/or $\delta$
- no master equation for level occupations
Nonequil. Green fct. approach

Renorm. spectral function of quantum dot level:

\[ \mathcal{A}(t, E) = A(1 - \partial_E \Lambda) + \Gamma \partial_E \text{Re} G_r \geq 0 \]

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

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

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

\[ d_t \mathcal{E}(t) = \sum_{\nu} \dot{\mathcal{Q}}_{\nu}(t) + \dot{\mathcal{W}} + \dot{\mathcal{W}}_c \]

\[ d_t S(t) = \dot{S}_i(t) + \sum_{\nu} \frac{\dot{Q}_\nu(t)}{T_\nu} \]

Esposito et al., PRL 2015
Extended level approach

Quantum thermodynamics of the driven resonant level model

Anton Bruch, Mark Thomas, Silvia Viola Kusminskiy, Felix von Oppen, and Abraham Nitzan

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

extended level

\[ q(\varepsilon) \rightarrow q_{\text{ex}}(\varepsilon) = A(\varepsilon) \]

\[
\Omega = -k_B T \int \frac{d\varepsilon}{2\pi} A \ln(1 + e^{-\beta(\varepsilon-\mu)})
\]
Scattering approach

PHYICAL REVIEW B 89, 161306(R) (2014)

Dynamical energy transfer in ac-driven quantum systems

María Florencia Ludovico, Jong Soo Lim, Michael Moskalets, Liliana Arrachea, and David Sánchez

We analyze the time-dependent energy and heat flows in a resonant level coupled to a fermionic continuum. The level is periodically forced with an external power source that supplies energy into the system. Based on the tunneling Hamiltonian approach and scattering theory, we discuss the different contributions to the total energy flux. We then derive the appropriate expression for the dynamical dissipation, in accordance with the fundamental principles of thermodynamics. Remarkably, we find that the dissipated heat can be expressed as a Joule law with a universal resistance that is constant at all times.
Landauer-Büttiker approach

- electronic transport as quantum scattering problem
  - quantum coherent transport
  - non-interacting electrons
  - equilibration occurs in reservoirs at infinity
Inside-outside duality

Particle number conservation:

change of particle number in scattering region
= balance of incoming & outgoing currents
von Neumann entropy \[ S[\rho] = -\text{Tr} (\rho \ln \rho) \]

conserved in coherent quantum dynamics \[ \rho \rightarrow U\rho U^+ \]

\[ \frac{ds}{dt} + I_{tot}^S = 0 \]

Bruch, Lewenkopf, FvO, PRL 120, 107701 (2018)
Conductance (zero $T$)

$$G = \frac{\text{d}I}{\text{d}V} = \frac{e^2}{h} T(E_F)$$

S-matrix

$$\begin{pmatrix} b_L \\ b_R \end{pmatrix} = S(E) \begin{pmatrix} a_L \\ a_R \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_L \\ a_R \end{pmatrix}$$

density of states per channel

$$\nu(E) = \frac{1}{2\pi \hbar \nu(E)}$$

current

$$I = e \int_{E_F}^{E_F+eV} \text{d}E \nu(E) \nu(E) \text{tr} \ t(E)t^+(E)$$

Quantum Thermodynamics
Resonant level model

\[ S = 1 + 2\pi i\nu_0 V \frac{1}{E - \epsilon_d + i\pi\nu_0 V^+ V} \]

Partial widths

\[ \Gamma_{L/R} = 2\pi |V_{L/R}|^2 \nu_0 \]

\[ V = \begin{pmatrix} V_L \\ V_R \end{pmatrix} \]

\[ G(E_F) = \frac{e^2}{h} \frac{\Gamma_L \Gamma_R}{(E_F - \epsilon_d)^2 + \left(\frac{\Gamma_L}{2} + \frac{\Gamma_R}{2}\right)^2} \]

\[ \frac{e^2}{h} \frac{4\Gamma_L \Gamma_R}{(\Gamma_L + \Gamma_R)^2} \]
Joule heating

\[ E_F + eV \]

right reservoir \( (I/e)(eV/2) = IV/2 \)

left reservoir \( (I/e)(eV/2) = IV/2 \)

Entropy production associated with Joule heating
\[ P=IV \] occurs entirely in the reservoirs.
Time-dependent scatterer generates excitations in the outgoing channels.

Entropy production is associated with equilibration of these excitations in the reservoirs.
Adiabatic approximation

Quasistatic processes: \( X(t) \) varies slowly so that one can use adiabatic approximation (expansion in powers of “velocity” \( \dot{X} \).
Adiabatic approximation

Change of S-matrix (or scattering phase $\theta$) is small during typical dwell time of electrons in scattering region:

$$\hbar \left| \frac{d\theta}{dt} \frac{d\theta}{dE} \right| \ll 1$$

Resonant level model:

$$\frac{d\theta}{dE} \sim \frac{1}{\Gamma}$$
Landauer-Büttiker approach

incoming channels

\[ \langle a^\dagger_\beta(\epsilon)a_\alpha(\epsilon') \rangle = \delta_{\alpha\beta}\delta(\epsilon - \epsilon')\phi^{\text{in}}(\epsilon) \]

with \( \phi^{\text{in}}(\epsilon) = f(\epsilon) \)

outgoing channels

\[
\phi^{\text{out}}_{\alpha\beta}(t, \epsilon) = \int_{-\infty}^{\infty} \frac{d\tilde{\epsilon}}{2\pi} e^{-i\tilde{\epsilon}t} \langle b^\dagger_\beta(\epsilon - \tilde{\epsilon}/2)b_\alpha(\epsilon + \tilde{\epsilon}/2) \rangle
\]

charge current

\[
I_\alpha(t) = e \int \frac{d\epsilon}{2\pi} \text{tr}_\alpha \{\phi^{\text{out}}(t, \epsilon) - \phi^{\text{in}}(\epsilon)\}
\]
Energy and heat current

**Energy current**

\[ I^E_\alpha(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \epsilon \text{tr}_c \{ \phi^{\text{out}}(t, \epsilon) - \phi^{\text{in}}(\epsilon) \} \]

**Heat current**

\[ I^{Q}_{\text{tot}}(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} (\epsilon - \mu) \text{tr}_c \{ \phi^{\text{out}}(t, \epsilon) - \phi^{\text{in}}(\epsilon) \} \]
Entropy per state (equilibrium)

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

Entropy current

\[ I_{\text{tot}}^S(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \text{tr}_c \left\{ \sigma[\phi^{\text{out}}(t, \epsilon)] - \sigma[\phi^{\text{in}}(\epsilon)] \right\} \]
S-matrix

\[
\left( \begin{array}{c}
  b_1(\epsilon) \\
  \vdots \\
  b_N(\epsilon)
\end{array} \right) = \int \frac{d\epsilon'}{2\pi} S(\epsilon, \epsilon') \left( \begin{array}{c}
  a_1(\epsilon') \\
  \vdots \\
  a_N(\epsilon')
\end{array} \right)
\]

adiabatic limit

\[
S(\epsilon, t) = S + \dot{X} A + ...
\]

\[
\phi^{\text{out}}(\epsilon, t) \approx \hat{I} f + \phi^{\text{out}(1)} + \phi^{\text{out}(2)}
\]

e.g. \[
\phi^{\text{out}(1)}(\epsilon, t) = i \dot{X} \partial_\epsilon f S \partial_X S^\dagger
\]

Brouwer, PRB 1998
Calculation

Expanding $\phi_{\text{out}}$ in powers of the velocity $\dot{X}$

$$\phi_{\text{out}} \simeq \hat{I} f + \phi_{\text{out}(1)} + \phi_{\text{out}(2)}$$

$$\sigma[\phi_{\text{out}}] \simeq \hat{I} \sigma[f] + \hat{I} \frac{d \sigma[f]}{df} (\phi_{\text{out}(1)} + \phi_{\text{out}(2)}) + \frac{1}{2} \hat{I} \frac{d^2 \sigma[f]}{df^2} (\phi_{\text{out}(1)})^2$$

$$I_{\text{tot}}^S = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \text{tr}_c \left\{ \frac{\epsilon - \mu}{T} (\phi_{\text{out}(1)} + \phi_{\text{out}(2)}) + \frac{1}{2T \partial_{\epsilon} f} (\phi_{\text{out}(1)})^2 \right\}$$

heat current/T

entropy production
Entropy production

\[ I_{\text{tot}}^S = \int_{-\infty}^{\infty} \frac{de}{2\pi} \text{tr}_c \left\{ \frac{\epsilon - \mu}{T} (\phi^{\text{out}(1)} + \phi^{\text{out}(2)}) + \frac{1}{2T\partial_c f} (\phi^{\text{out}(1)})^2 \right\} \]

\[ I_{\text{tot}}^S = \frac{I_{\text{tot}}^Q}{T} - \frac{\dot{W}^{(2)}}{T} \]

Inside-outside duality:

\[ \dot{S}_i = \frac{ds}{dt} = \frac{\dot{Q}}{T} + \frac{\dot{W}^{(2)}}{T} \]
Entropy production

\[ I_{\text{tot}}^S = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \text{tr}_c \left\{ \frac{\epsilon - \mu}{T} \left( \phi_{\text{out}(1)} + \phi_{\text{out}(2)} \right) + \frac{1}{2T\partial_\epsilon f} (\phi_{\text{out}(1)})^2 \right\} \]

entropy production

explicit calculation in gradient expansion

\[ \phi_{\text{out}(1)}(\epsilon, t) = i\hat{X}\partial_\epsilon f S\partial_X S^\dagger \]

Brouwer, PRB 1998

\[ \dot{S}_i = \frac{\dot{X}^2}{2T} \int \frac{d\epsilon}{2\pi} (-\partial_\epsilon f) \text{tr}_c (\partial_X S^+ \partial_X S) \geq 0 \]
Resonant level model

\[ \dot{S}_i = \frac{\dot{\epsilon}_d^2}{2T} \int \frac{d\epsilon}{2\pi} (-\partial_\epsilon f) A^2 \]

\[ A(\epsilon) = \frac{\Gamma}{(\epsilon - \epsilon_d)^2 + (\Gamma/2)^2} \]

Bruch, Thomas, Kusminskiy, FvO, Nitzan, PRB 93, 115318 (2016)
Towards an interpretation

Parameter $X(t)$ is dynamical variable with its own (classical) dynamics.

Electrons (fast) exert forces on mechanical degrees of freedom of nanotube (slow).

displacement $X$ of nanotube

change in dot level $\varepsilon_d(X)$
Adiabatic approximation

Coupling fast quantum system (electrons) to slow degree(s) of freedom (nuclei)

- compute electronic levels for fixed nuclear coordinates
- electrons exert potential (Born-Oppenheimer) force on nuclei

$E = - \nabla_R E$

R: internuclear distance
Beyond Born-Oppenheimer

Chaotic classical and half-classical adiabatic reactions: geometric magnetism and deterministic friction

By M. V. Berry and J. M. Robbins


\[ \hat{H}(\mathbf{R}(t)) \ket{\psi(t)} = i\hbar \ket{\dot{\psi}(t)} \]

next order in \( \dot{\mathbf{R}} \)

quantum system acquires Berry’s phase

slow system subject to velocity-dependent force

\[ \gamma_n(C) = i \oint_C \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle \cdot d\mathbf{R} \]

\[ \delta F_\nu = -\sum_{\nu'} \gamma_{\nu\nu'} \dot{X}_{\nu'} \]
Friction and fluctuating force

**Berry:** discrete quantum system → no friction
(but geometric magnetism)

**here:** quantum mechanical scattering system
w/ continuous spectrum → friction appears naturally

Fluctuation-dissipation theorem:
fluctuating Langevin force in addition to friction
Langevin dynamics

\[ M_{\nu} \ddot{X}_{\nu} + \frac{\partial U}{\partial X_{\nu}} = F_{\nu} - \sum_{\nu'} \gamma_{\nu\nu'} \dot{X}_{\nu'} + \xi_{\nu} \]

- Born-Oppenheimer force \( F_{\nu} \)
- velocity-dependent force \(-\sum \gamma_{\nu\mu} X_{\mu}\)
- Langevin force \( \xi_{\nu} : \quad \langle \xi_{\nu}(t) \xi_{\nu'}(t') \rangle = D_{\nu\nu'}(X) \delta(t - t') \)
Friction

\[ F_{fric} = -\gamma \dot{X} \quad \gamma = \int \frac{d\epsilon}{4\pi} (-\partial_{\epsilon} f) \text{tr} \left\{ \frac{\partial S^+}{\partial X} \frac{\partial S}{\partial X} \right\} \]

Dissipated power:

\[ P = T \dot{S_i} = \gamma \dot{X}^2 \]

Entropy production is just associated with frictional force that has to be overcome to change the system parameters.

Bode, Kusminskiy, Egger, FvO, PRL 2011
Thomas, Karzig, Kusminskiy, Zarand, FvO, PRB 2012
Gilbert damping

Landau-Lifshitz-Gilbert equation:

\[
\frac{1}{\gamma} \frac{dM}{d\tau} = - M \times H_{\text{eff}} + M \times \left[ \hat{G}(M) \frac{dM}{d\tau} \right]
\]

Gilbert coefficient:

\[
G_{ij}(m) = \frac{\gamma^2 \hbar}{4\pi} \text{Re} \left\{ \text{Tr} \left[ \frac{\partial S}{\partial m_i} \frac{\partial S^\dagger}{\partial m_j} \right] \right\}
\]
Born-Oppenheimer force

adiabatic S-matrix: $S(\epsilon, X)$

$$M_v \ddot{X}_v + \frac{\partial U}{\partial X_v} = F_v - \sum_{\nu'} \gamma_{\nu\nu'} \dot{X}_{\nu'} + \xi_v$$

$$F_v(X) = \sum_{\alpha} \int \frac{d\epsilon}{2\pi i} f_\alpha \operatorname{Tr}\left( \Pi_\alpha S^\dagger \frac{\partial S}{\partial X_v} \right)$$
Thermal equilibrium

Born-Oppenheimer:

\[ F_\alpha(X_t) = -\sum_i f(E_t^i) \partial_\alpha E_t^i \]

Friedel sum rule:

\[ N(\epsilon, X_t) = \int_{-\infty}^{\epsilon} d\epsilon' \nu(\tilde{\epsilon}', X_t) \]

\[ = \frac{1}{2\pi i} \text{tr} \{ \ln S_t(\epsilon) \} \]

\[ F_\alpha(X_t) = \int_{-\infty}^{\mu} d\epsilon \partial_\alpha N(\epsilon, X_t) = \int_{-\infty}^{\mu} \frac{d\epsilon}{2\pi i} \text{tr} \left\{ S_t^\dagger(\epsilon) \partial_\alpha S_t(\epsilon) \right\} \]

- force is conservative in thermal equilibrium
Out of equilibrium

Out-of-equilibrium conductor:

Born-Oppenheimer force generally non-conservative

Work performed on mechanical modes per cycle

\[ W_{\text{out}} = \oint d\mathbf{X} \cdot \mathbf{F}(\mathbf{X}) \]

Linear response:

\[ W_{\text{out}} = \frac{eV}{2} \oint d\mathbf{X} \cdot \int \frac{d\epsilon}{2\pi i} \left( -\frac{\partial f}{\partial \epsilon} \right) \text{Tr} \left\{ (\Pi_L - \Pi_R) S^\dagger \frac{\partial S}{\partial \mathbf{X}} \right\} \]

see also: Todorov et al. 2008, Lü et al. 2010
Relation to quantum pumping

Quantum pumping of charge $Q_p$ through mesoscopic conductor

$$Q_p = e \oint d\mathbf{X} \cdot \int \frac{d\epsilon}{4\pi i} \left( -\frac{\partial f}{\partial \epsilon} \right) \text{Tr} \left\{ (\Pi_L - \Pi_R) S^\dagger \frac{\partial S}{\partial \mathbf{X}} \right\}$$

$W_{out} = Q_p V$

Non-conservative
Born-Oppenheimer force

Quantum pumping
of charge

Brouwer 1998
Adiabatic quantum motor

Motor pumps charge with voltage drop and converts the electrical energy gain into motor action.

one motor revolution

pumped charge $Q_p$

electrical energy gain of motor per cycle $Q_p V$

Quantum Thermodynamics
Archimedes' screw

Archimedes' screw, also called the Archimedean screw or screwpump, is a machine historically used for transferring water from a low-lying body of water into irrigation ditches.

Reverse action

If water is poured into the top of an Archimedes' screw, it will force the screw to rotate. The rotating shaft can then be used to drive an electric generator. Such an installation has the same benefits as using the screw for pumping: the ability to handle very dirty water and widely varying rates of flow at high efficiency. Settle Hydro and Torrs Hydro are two reverse screw micro hydro schemes operating in England. As a generator the screw is good at low heads, commonly found in English rivers, including the Thames powering Windsor Castle.\(^8\)[9]
Topological (Thouless) motor

Quantization of particle transport

D. J. Thouless

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sliding periodic potential: pumped charge is quantized when Fermi energy is in energy gap

R. Bustos Marun, G. Refael, FvO, PRL 2013
Dissipation of Thouless motor

Friction force:
\[ \gamma_{\text{int}} = \frac{\hbar}{4\pi} \text{tr} \left[ \left( \frac{\partial S^\dagger}{\partial \theta} \right) \left( \frac{\partial S}{\partial \theta} \right) \right] \]

\[ \gamma_{\text{int}} = \left( \frac{\hbar}{2\pi e} \right) Q_p \]

quantum dissipation

\[ (x + \gamma_{\text{int}}) \dot{\theta} = \frac{Q_p V}{2\pi} \]

\[ I = \frac{Q_p \dot{\theta}}{2\pi} \]

\[ V = \frac{h}{e^2 I} \]

R. Bustos Marun, G. Refael, FvO, PRL 2013
Conclusions and outlook

- scattering theory approach to quantum thermodynamics of electronic nano-engines
- entropy production and frictional force
- validity: arbitrary non-interacting, fully coherent electron systems with adiabatic parameter variations
- extensions: voltage or temperature bias, beyond adiabaticity, electron-electron interactions, application to nano-engines