



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
Phys. Rev. B **93**, 115318 (2016)

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



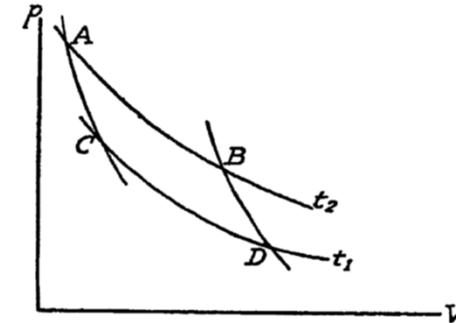
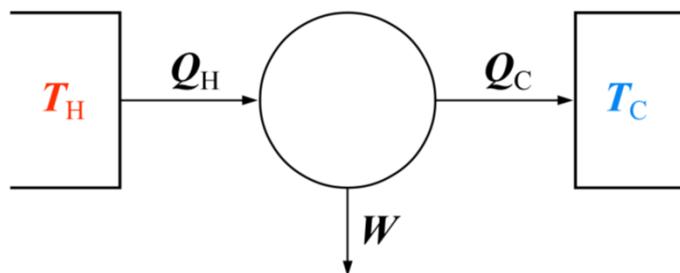
➤ Outside approach

*Landauer-Büttiker approach to strongly coupled quantum thermodynamics:
inside-outside duality of entropy evolution*
Phys. Rev. Lett. **120**, 107701 (2018)

w/ Anton Bruch & Caio Lewenkopf



Classic(al) heat engine



First law $dU = dW + dQ$

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

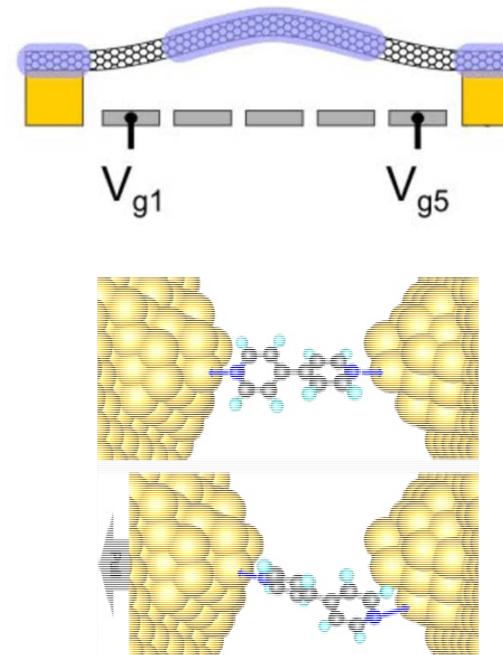
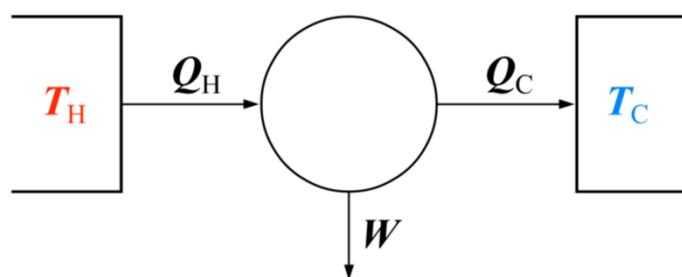
Carnot 1824



max. efficiency $\eta_C = \frac{T_H - T_C}{T_H}$



Nano-engine



First law

$$dU = dW + dQ$$

Second law

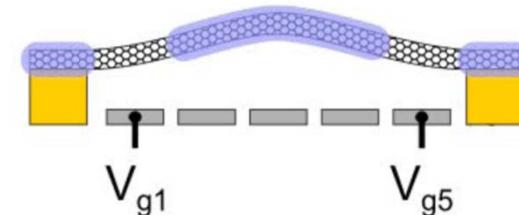
$$\frac{dS}{dt} = \frac{\dot{Q}}{T} + \dot{\mathcal{S}}_i \quad \dot{\mathcal{S}}_i \geq 0$$

- 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**

Entropy production



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

- 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

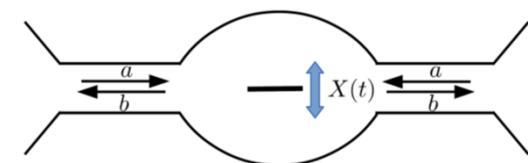
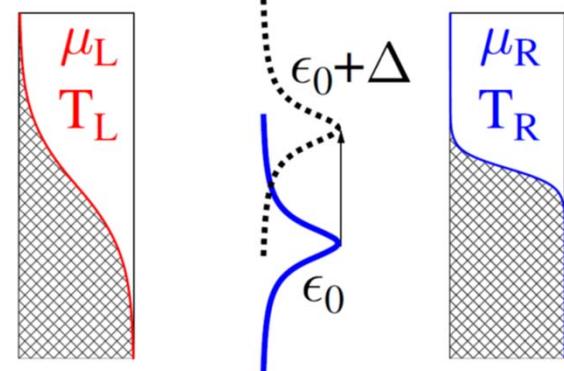
$$H_D = \varepsilon_d(t) d^\dagger d$$

leads

$$H_B = \sum_k \varepsilon_k c_k^\dagger c_k$$

dot-lead coupling

$$H_V = \sum_k (V_k d^\dagger c_k + \text{H.c.})$$



- non-interacting electrons
- adiabatic variation of ε_d, V_k (slow compared to Γ)
- non-equilibrium beyond quasi-static limit

Strong system-reservoir coupling

PRL 114, 080602 (2015)

PHYSICAL REVIEW LETTERS

week ending
27 FEBRUARY 2015



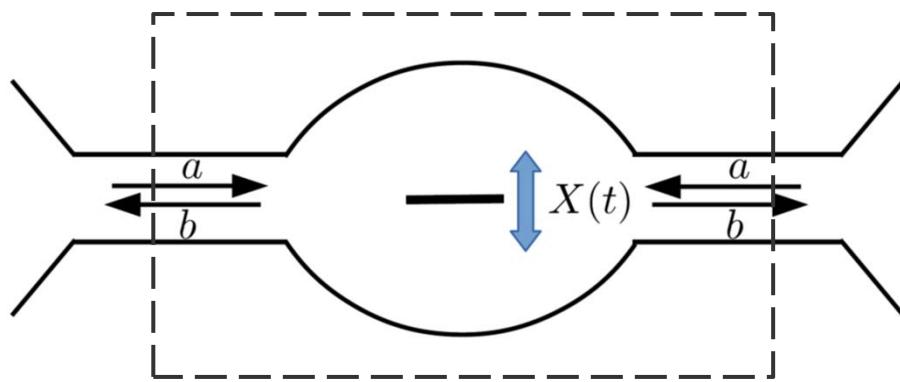
Quantum Thermodynamics: A Nonequilibrium Green's Function Approach

Massimiliano Esposito

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(Received 5 November 2014; revised manuscript received 22 December 2014; published 25 February 2015)*



- full quantum coherence
- strong coupling:
 $\Gamma \gg T$ and/or δ
- no master equation
for level occupations

Renorm. spectral function
of quantum dot level:

$$\mathcal{A}(t, E) = A(1 - \partial_E \Lambda) + \Gamma \partial_E \text{Re} G^r \geq 0$$

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

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

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

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

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

Esposito *et al.*, PRL 2015

Extended level approach

PHYSICAL REVIEW B **93**, 115318 (2016)

Quantum thermodynamics of the driven resonant level model

Anton Bruch,¹ Mark Thomas,¹ Silvia Viola Kusminskiy,¹ Felix von Oppen,¹ and Abraham Nitzan^{1,2,3}

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

extended level



$$\varrho(\epsilon) \rightarrow \varrho_{ex}(\epsilon) = A(\epsilon)$$

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

Scattering approach

PHYSICAL REVIEW B **89**, 161306(R) (2014)

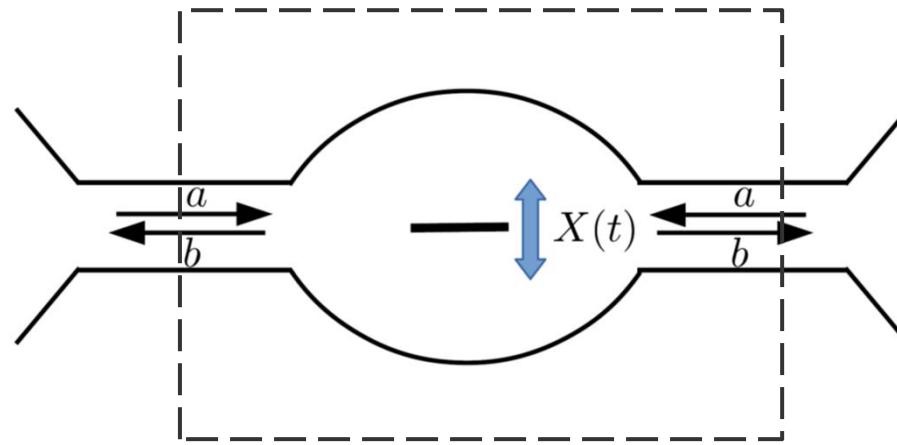
Dynamical energy transfer in ac-driven quantum systems

María Florencia Ludovico,^{1,*} Jong Soo Lim,^{2,3,*} Michael Moskalets,⁴ Liliana Arrachea,¹ and David Sánchez^{2,5}

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.

Focus on currents deep in the electrodes rather than quantities associated with quantum dot

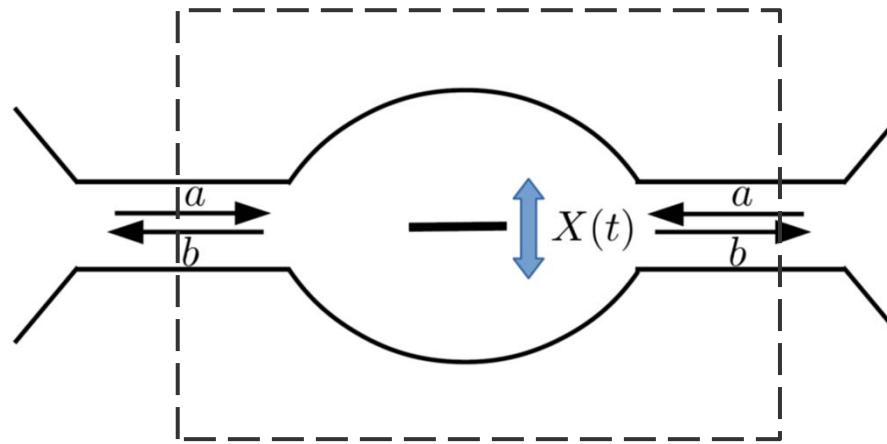
Landauer-Büttiker approach



electronic transport as quantum scattering problem

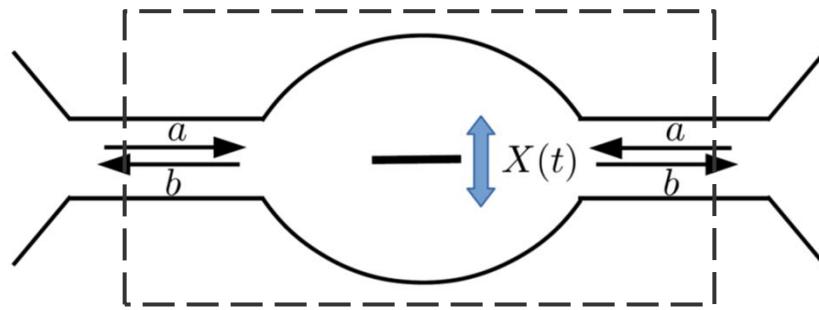
- quantum coherent transport
- non-interacting electrons
- equilibration occurs in reservoirs at infinity

Inside-outside duality



Particle number conservation:

change of particle number in scattering region
= balance of incoming & outgoing currents



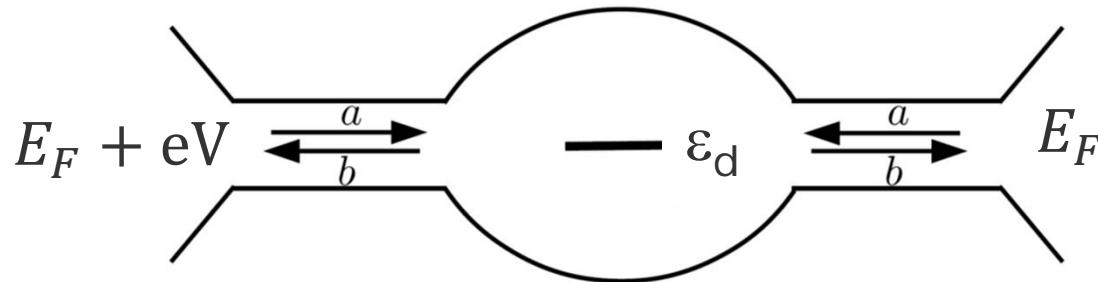
von Neumann entropy $\mathbf{S}[\rho] = -\text{Tr}(\rho \ln \rho)$

conserved in coherent quantum dynamics $\varrho \rightarrow U\varrho U^+$

$$\frac{ds}{dt} + I_{\text{tot}}^S = 0$$

Bruch, Lewenkopf, FvO, PRL 120, 107701 (2018)

Conductance (zero T)



$$G = \frac{dI}{dV} = \frac{e^2}{h} T(E_F)$$

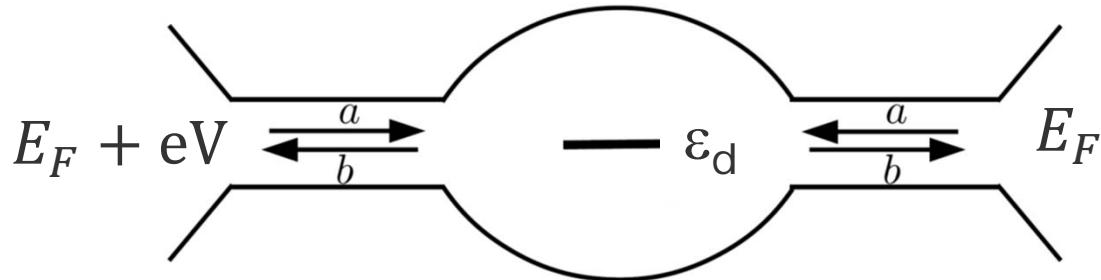
S-matrix $\begin{pmatrix} b_L \\ b_R \end{pmatrix} = S(E) \begin{pmatrix} a_L \\ a_R \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_L \\ a_R \end{pmatrix}$

density of states per channel

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

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

Resonant level model



Partial widths

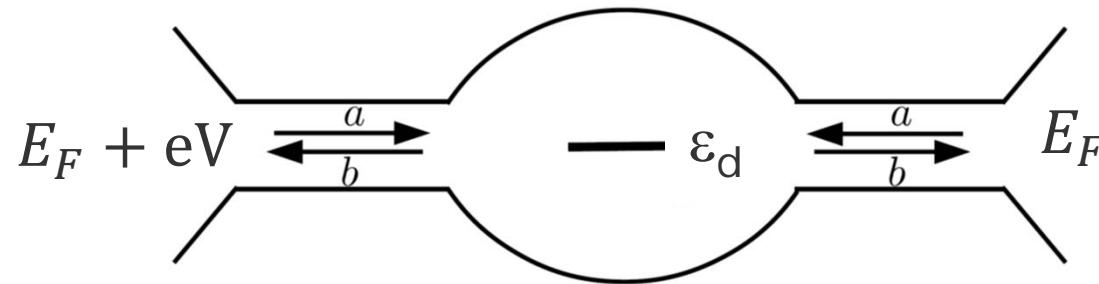
$$\Gamma_{L/R} = 2\pi |V_{L/R}|^2 \nu_0$$

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

$$V = \begin{pmatrix} V_L \\ V_R \end{pmatrix}$$

$$G(E_F) = \frac{e^2}{h} \frac{\Gamma_L \Gamma_R}{(E_F - \epsilon_d)^2 + \left(\frac{\Gamma_L}{2} + \frac{\Gamma_R}{2}\right)^2} \xrightarrow{E_F=\epsilon_d} \frac{e^2}{h} \frac{4\Gamma_L \Gamma_R}{(\Gamma_L + \Gamma_R)^2}$$

Joule heating



right reservoir

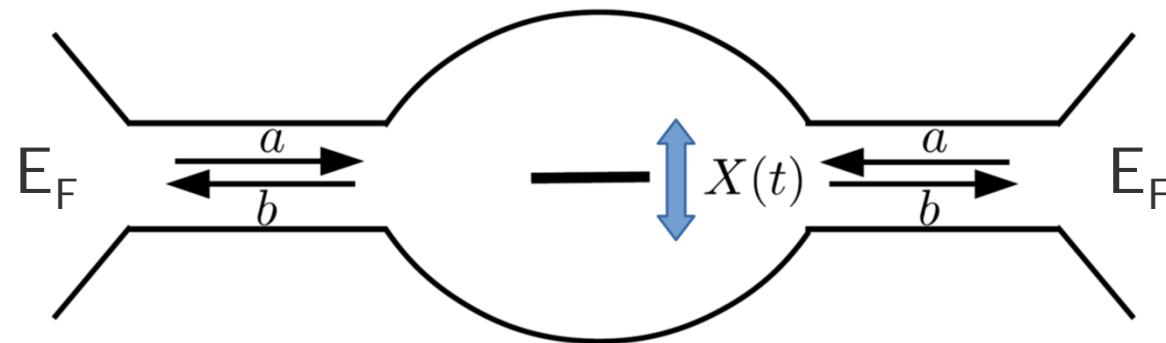
$$(I/e)(eV/2) = IV/2$$

left reservoir

$$(I/e)(eV/2) = IV/2$$

Entropy production associated with Joule heating
 $P=IV$ occurs entirely in the reservoirs.

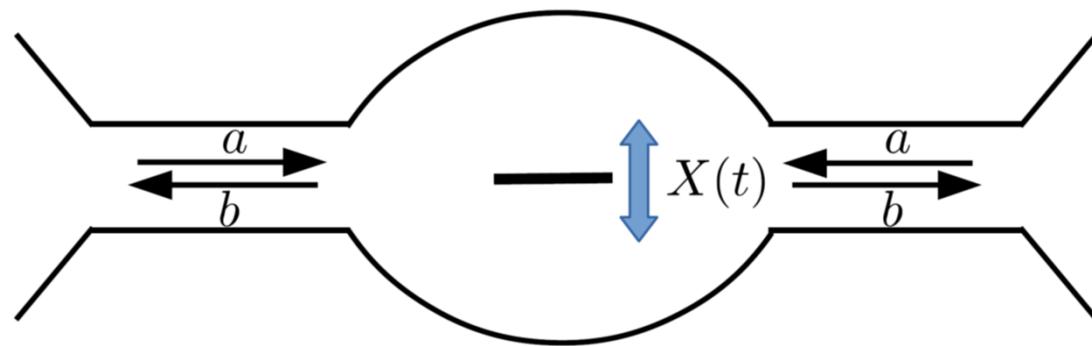
Time-dependent scatterer



Time-dependent scatterer generates excitations in the outgoing channels.

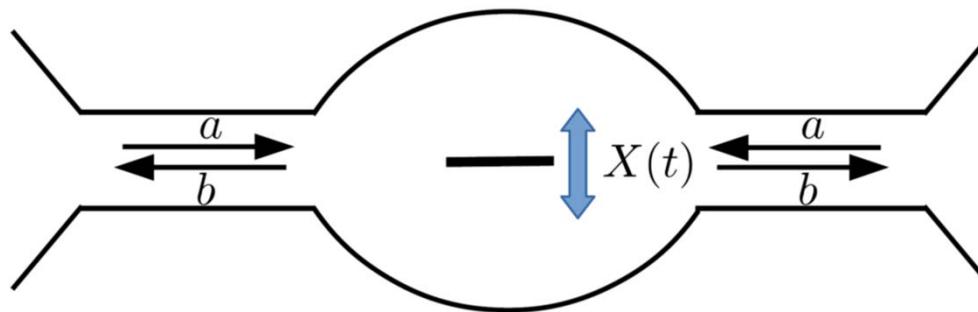
Entropy production is associated with equilibration of these excitations in the reservoirs.

Adiabatic approximation



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

Adiabatic approximation

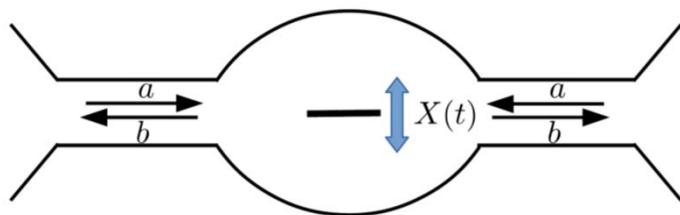


Change of S-matrix (or scattering phase θ) is small during typical dwell time of electrons in scattering region:

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

Resonant level model: $\frac{d\theta}{dE} \sim \frac{1}{\Gamma}$

Landauer-Büttiker approach



incoming channels

$$\langle a_\beta^\dagger(\epsilon) a_\alpha(\epsilon') \rangle = \delta_{\alpha\beta} \delta(\epsilon - \epsilon') \phi^{\text{in}}(\epsilon)$$

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

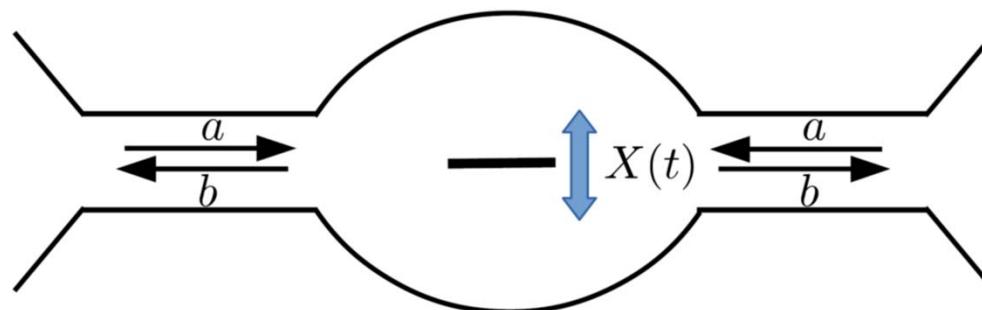
outgoing channels

$$\phi_{\alpha\beta}^{\text{out}}(t, \epsilon) = \int_{-\infty}^{\infty} \frac{d\tilde{\epsilon}}{2\pi} e^{-i\tilde{\epsilon}t} \langle b_\beta^\dagger(\epsilon - \tilde{\epsilon}/2) b_\alpha(\epsilon + \tilde{\epsilon}/2) \rangle$$

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

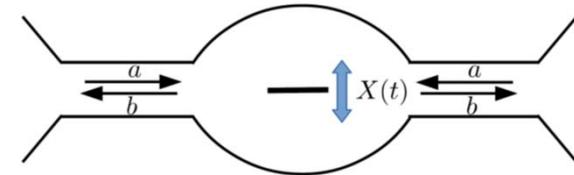
$$I_\alpha^E(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \epsilon \text{tr}_c \{ \phi^{\text{out}}(t, \epsilon) - \phi^{\text{in}}(\epsilon) \}$$

heat current

$$I_{\text{tot}}^Q(t) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} (\epsilon - \mu) \text{tr}_c \{ \phi^{\text{out}}(t, \epsilon) - \phi^{\text{in}}(\epsilon) \}$$

Entropy current

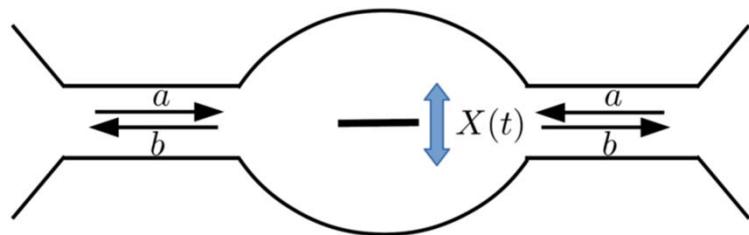
Entropy per state (equilibrium)



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

Entropy current

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



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

adiabatic limit

$$\left[\begin{array}{l} \mathcal{S}(\epsilon, t) = S + \dot{X}A + \dots \\ \phi^{\text{out}} \simeq \hat{I}f + \phi^{\text{out}(1)} + \phi^{\text{out}(2)} \end{array} \right]$$

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

Buttiker, Thomas, Pretre, Z. Phys. B 1994
Brouwer, PRB 1998

Calculation

Expanding ϕ_{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

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



$$I_{\text{tot}}^S = \frac{I_{\text{tot}}^Q}{T} - \frac{\dot{W}^{(2)}}{T} \quad \text{strictly negative}$$

Inside-outside duality:

$$\boxed{\frac{ds}{dt} = \frac{\dot{Q}}{T} + \frac{\dot{W}^{(2)}}{T}}$$

\dot{S}_i

Entropy production

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

entropy production

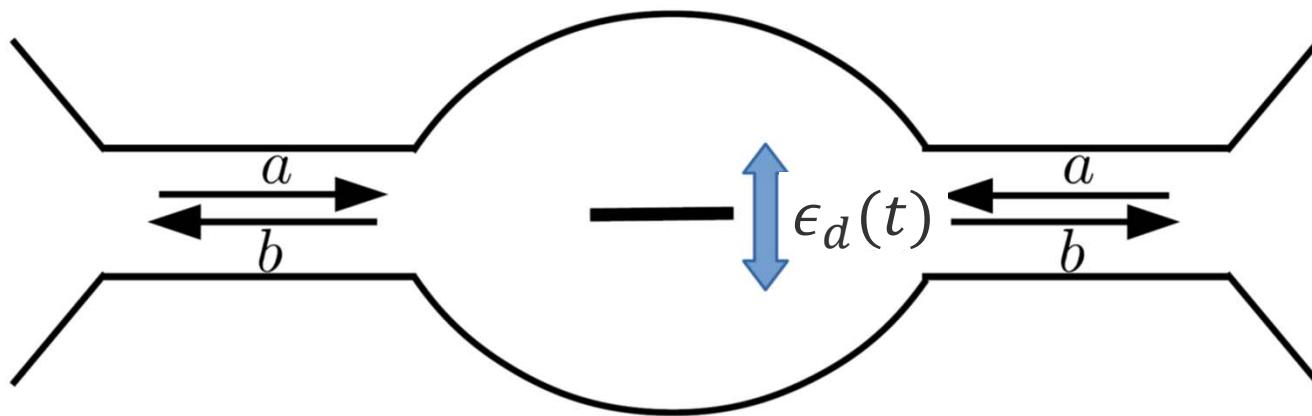
explicit calculation in gradient expansion

$$\phi^{\text{out}(1)}(\epsilon, t) = i \dot{X} \partial_\epsilon f S \partial_X S^\dagger$$

Buttiker, Thomas, Pretre, Z. Phys. B 1994
Brouwer, PRB 1998

$$\dot{S}_i = \frac{\dot{X}^2}{2T} \int \frac{d\epsilon}{2\pi} (-\partial_\epsilon f) \text{tr}_c (\partial_X S^\dagger \partial_X S) \geq 0$$

Resonant level model

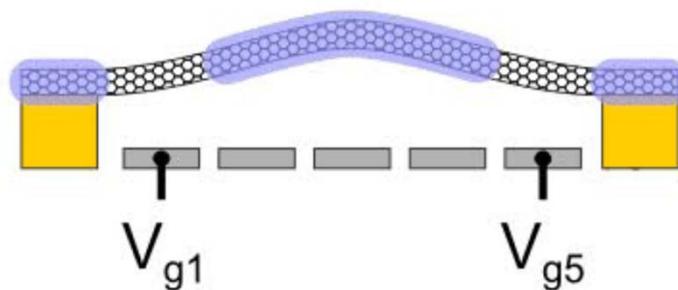


$$\dot{S}_i = \frac{\dot{\epsilon}_d^2}{2T} \int \frac{d\epsilon}{2\pi} (-\partial_\epsilon f) A^2$$

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

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

Towards an interpretation



displacement \mathbf{X} of nanotube



change in dot level $\varepsilon_d(\mathbf{X})$

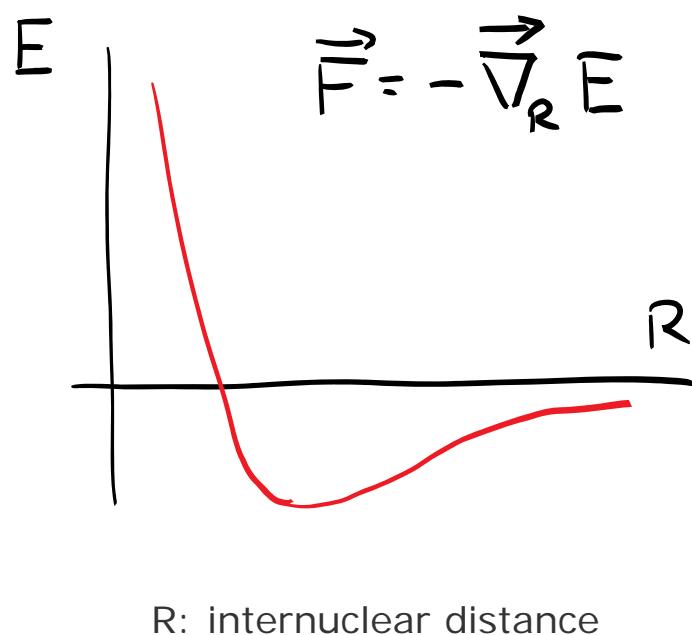
- Parameter $\mathbf{X}(t)$ is dynamical variable with its own (classical) dynamics.
- Electrons (fast) exert forces on mechanical degrees of freedom of nanotube (slow).

1927

Nº 20

ANNALEN DER PHYSIK VIERTE FOLGE. BAND 84

1. Zur Quantentheorie der Moleküle;
von M. Born und R. Oppenheimer



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

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

BY M. V. BERRY AND J. M. ROBBINS

Proc. R. Soc. Lond. A (1993) **442**, 659–672

$$\hat{H}(\mathbf{R}(t)) |\psi(t)\rangle = i\hbar |\dot{\psi}(t)\rangle$$



next order in $\dot{\mathbf{R}}$



quantum system acquires
Berry's phase

slow system subject to
velocity-dependent force

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

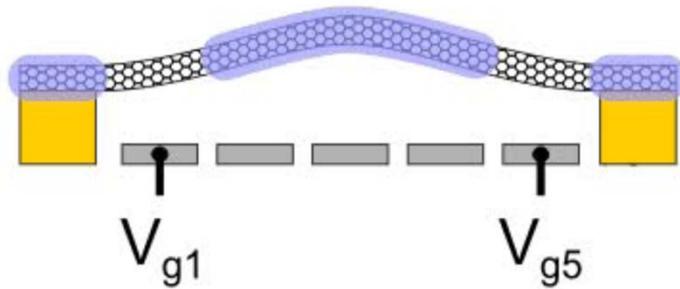
$$\delta F_\nu = - \sum_{\nu'} \gamma_{\nu\nu'} \dot{X}_{\nu'}$$

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_ν
- velocity-dependent force $-\sum \gamma_{\nu\mu} \dot{X}_\mu$
- Langevin force ξ_ν : $\langle \xi_\nu(t) \xi_{\nu'}(t') \rangle = D_{\nu\nu'}(\mathbf{X}) \delta(t - t')$

$$F_{fric} = -\gamma \dot{X}$$

$$\gamma = \int \frac{d\epsilon}{4\pi} (-\partial_\epsilon f) \text{tr} \left\{ \frac{\partial S^+}{\partial X} \frac{\partial S^-}{\partial X} \right\}$$

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

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.

Gilbert damping

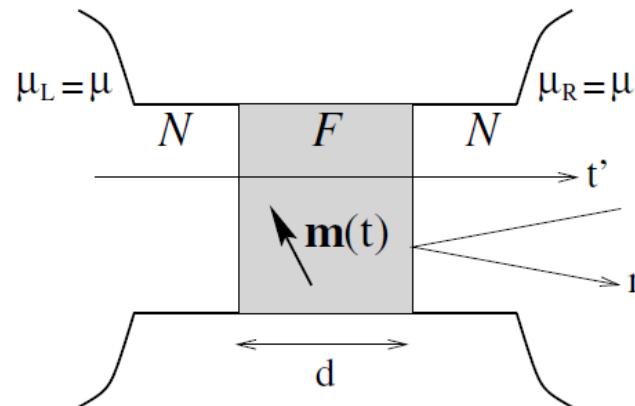
PRL 101, 037207 (2008)

PHYSICAL REVIEW LETTERS

week ending
18 JULY 2008

Scattering Theory of Gilbert Damping

Arne Brataas,^{1,*} Yaroslav Tserkovnyak,² and Gerrit E. W. Bauer³



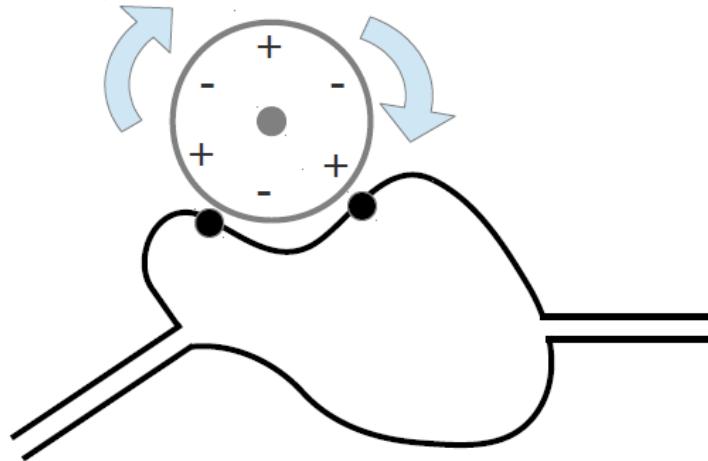
Landau-Lifshitz-Gilbert
equation:

$$\frac{1}{\gamma} \frac{d\mathbf{M}}{d\tau} = -\mathbf{M} \times \mathbf{H}_{\text{eff}} + \mathbf{M} \times \left[\frac{\tilde{G}(\mathbf{M})}{\gamma^2 M_s^2} \frac{d\mathbf{M}}{d\tau} \right]$$

Gilbert coefficient:

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

Born-Oppenheimer force



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

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

Born-Oppenheimer force:

$$F_\nu(\mathbf{X}) = \sum_\alpha \int \frac{d\epsilon}{2\pi i} f_\alpha \text{Tr} \left(\Pi_\alpha S^\dagger \frac{\partial S}{\partial X_\nu} \right)$$

Born-Oppenheimer: $F_\alpha(\mathbf{X}_t) = - \sum_i f(E_t^i) \partial_\alpha E_t^i$

Friedel sum rule:
$$\begin{aligned} N(\varepsilon, \mathbf{X}_t) &= \int_{-\infty}^{\varepsilon} d\varepsilon' \nu(\bar{\varepsilon'}, \mathbf{X}_t) \\ &= \frac{1}{2\pi i} \text{tr} \{ \ln S_t(\varepsilon) \} \end{aligned}$$

$$F_\alpha(\mathbf{X}_t) = \int_{-\infty}^{\mu} d\varepsilon \partial_\alpha N(\varepsilon, \mathbf{X}_t) = \int_{-\infty}^{\mu} \frac{d\varepsilon}{2\pi i} \text{tr} \left\{ S_t^\dagger(\varepsilon) \partial_\alpha S_t(\varepsilon) \right\}$$

- force is conservative in thermal equilibrium

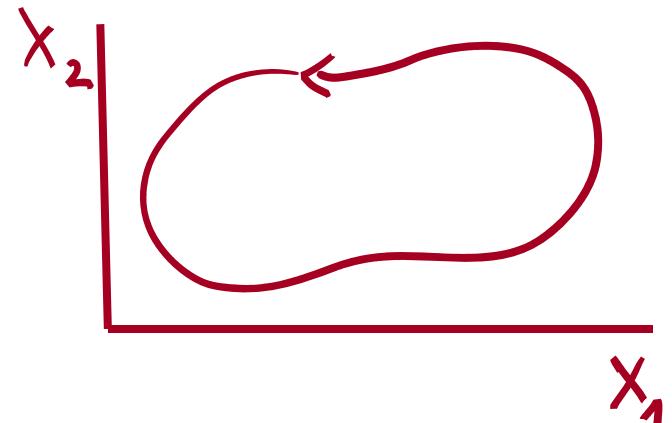
Out-of-equilibrium conductor:

Born-Oppenheimer force generally non-conservative

see also: Todorov et al. 2008, Lü et al. 2010

Work performed on mechanical modes per cycle

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



Linear response:

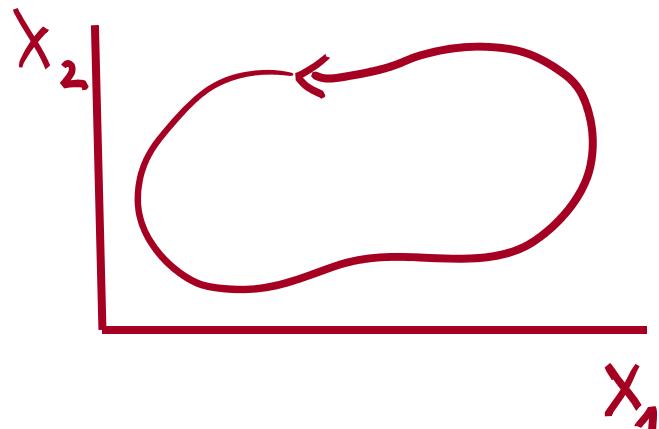
$$W_{\text{out}} = \frac{eV}{2} \oint d\mathbf{X} \cdot \int \frac{d\epsilon}{2\pi i} \left(-\frac{\partial f}{\partial \epsilon} \right) \text{Tr} \left\{ (\Pi_L - \Pi_R) S^\dagger \frac{\partial S}{\partial \mathbf{X}} \right\}$$

Relation to quantum pumping

quantum pumping of charge Q_p through mesoscopic conductor

Brouwer 1998

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



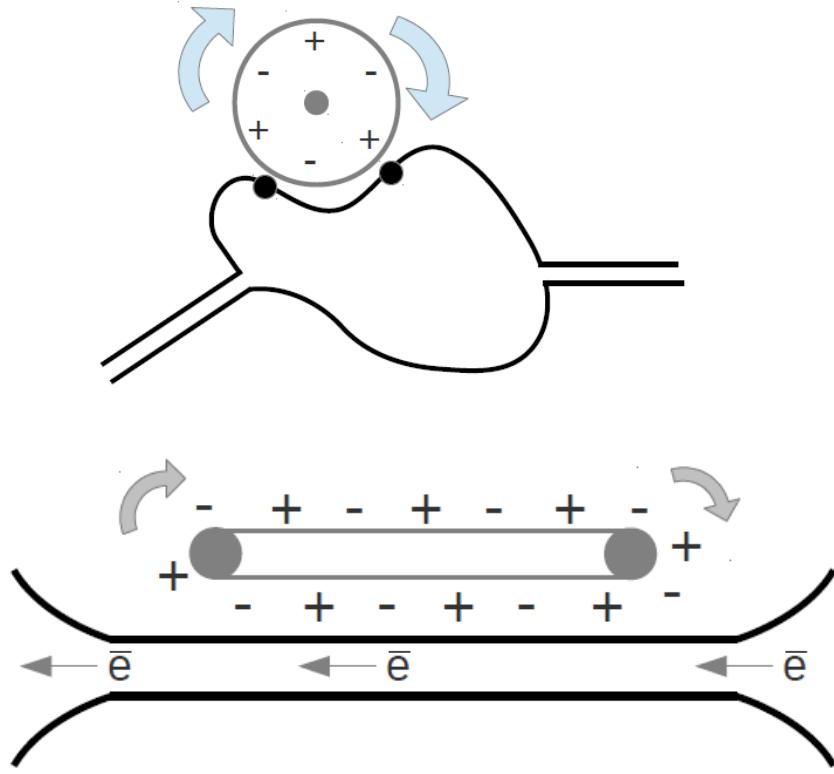
non-conservative
Born-Oppenheimer force



$$W_{\text{out}} = Q_p V$$

quantum pumping
of charge

Adiabatic quantum motor



one motor revolution



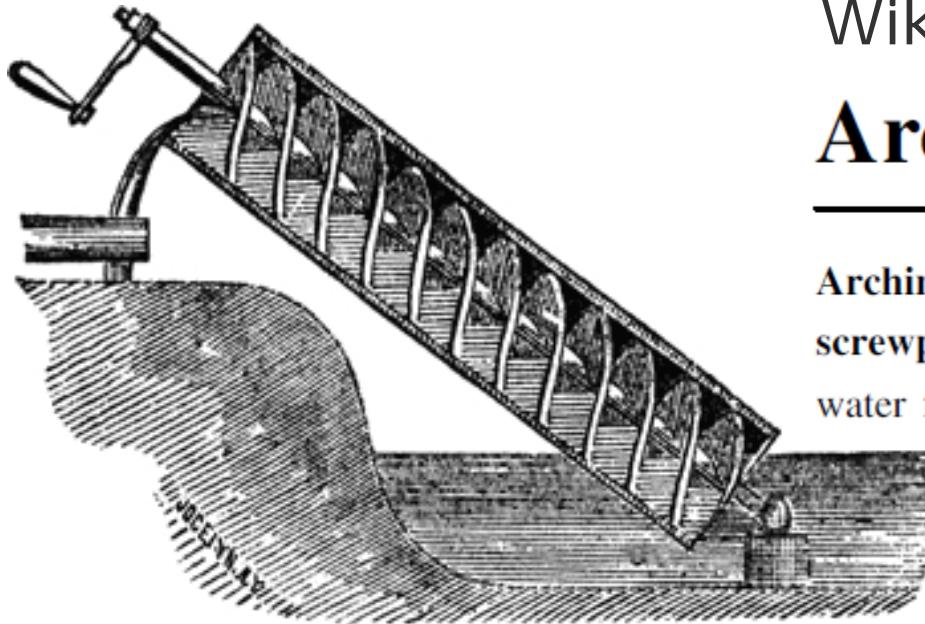
pumped charge Q_p



electrical energy gain
of motor per cycle

$$Q_p V$$

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



Wikipedia **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

PHYSICAL REVIEW B

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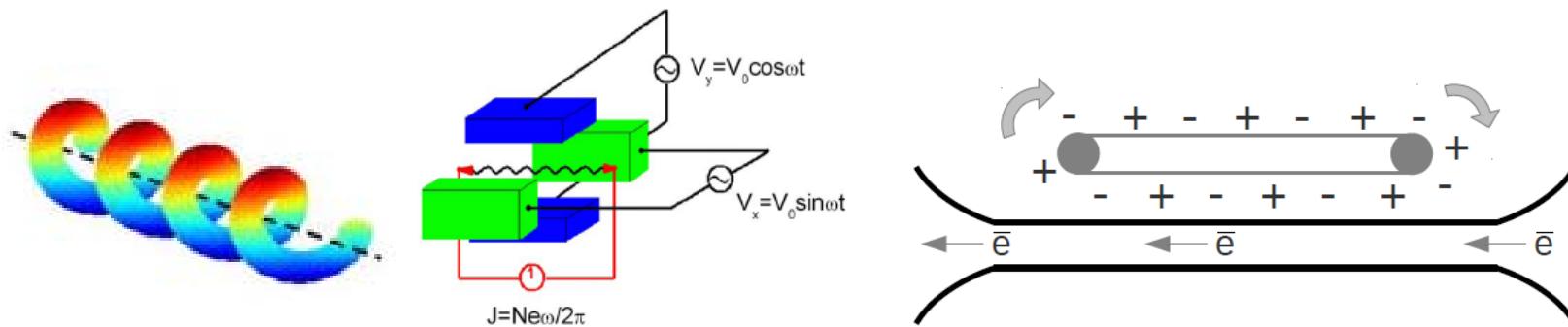
15 MAY 1983

Quantization of particle transport

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

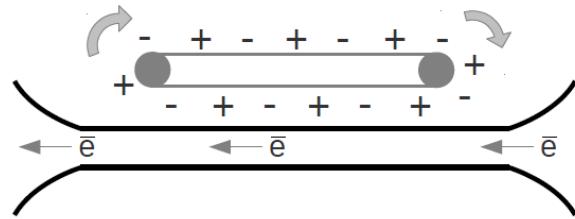


X.-L. Qi, S.C. Zhang PRB 2009

R. Bustos Marun, G. Refael, FvO, PRL 2013

Dissipation of Thouless motor

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



$$\gamma_{\text{int}} = (\hbar/2\pi e)Q_p$$

quantum dissipation

$$\cancel{X} + \gamma_{\text{int}}) \dot{\theta} = \frac{Q_p V}{2\pi}$$

$$I = \frac{Q_p \dot{\theta}}{2\pi}$$

$$V = \frac{h}{e^2} I$$

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

A. Bruch, M. Thomas, S. Kusminskiy, FvO, A. Nitzan, Phys. Rev. B 93, 115318 (2016)
A. Bruch, C. Lewenkopf, FvO, Phys. Rev. Lett. 120, 107701 (2018)
R. Bustos Marun, G. Refael, FvO, Phys. Rev. Lett 111, 060802 (2013)