DYNAMICS OF THE ENERGY TRANSPORT AND HEAT PRODUCTION IN ADIABATICALLY DRIVEN QUANTUM DOTS AND THE ROLE OF THE ENERGY REACTANCE

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KITP - 2018




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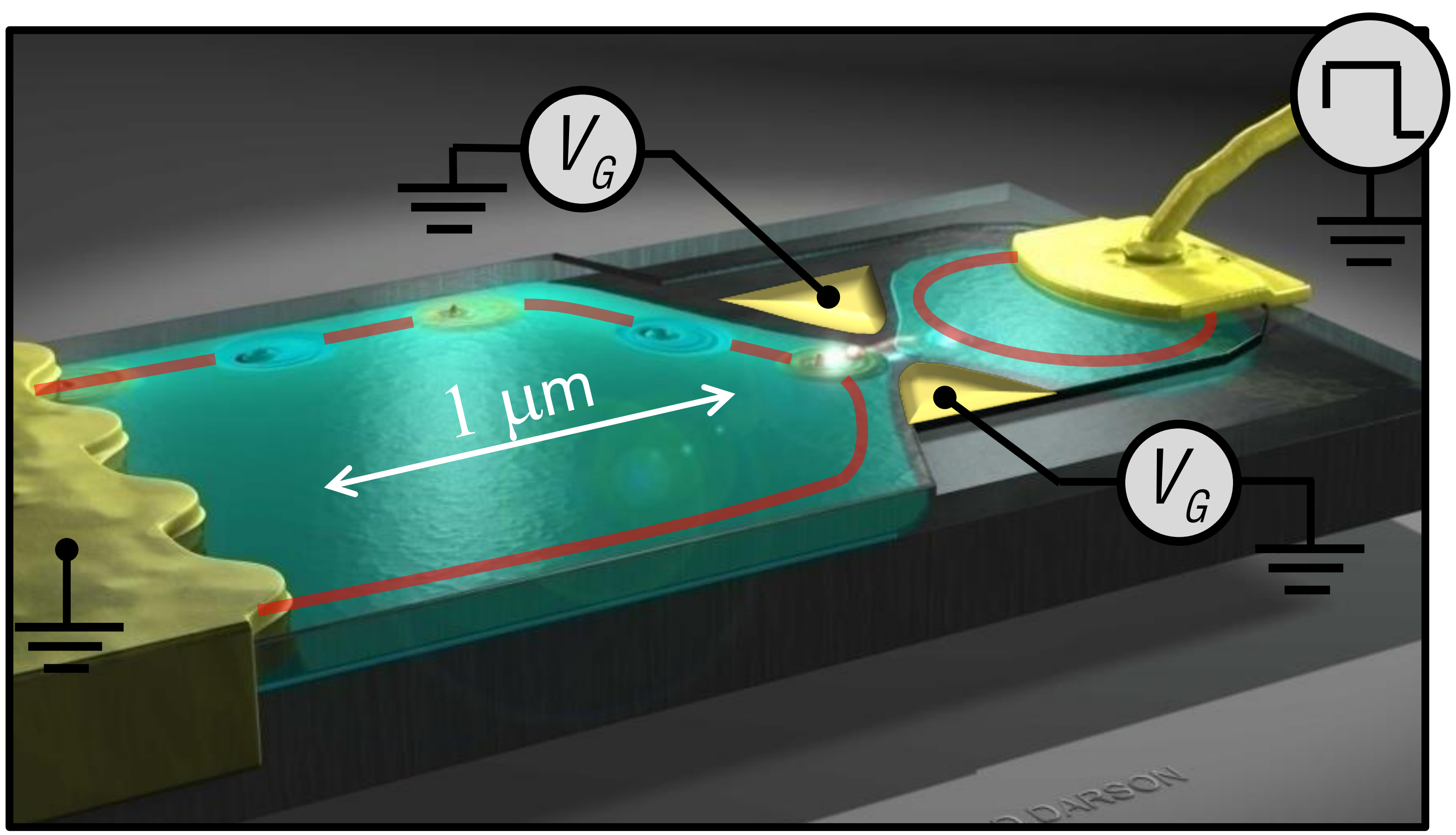
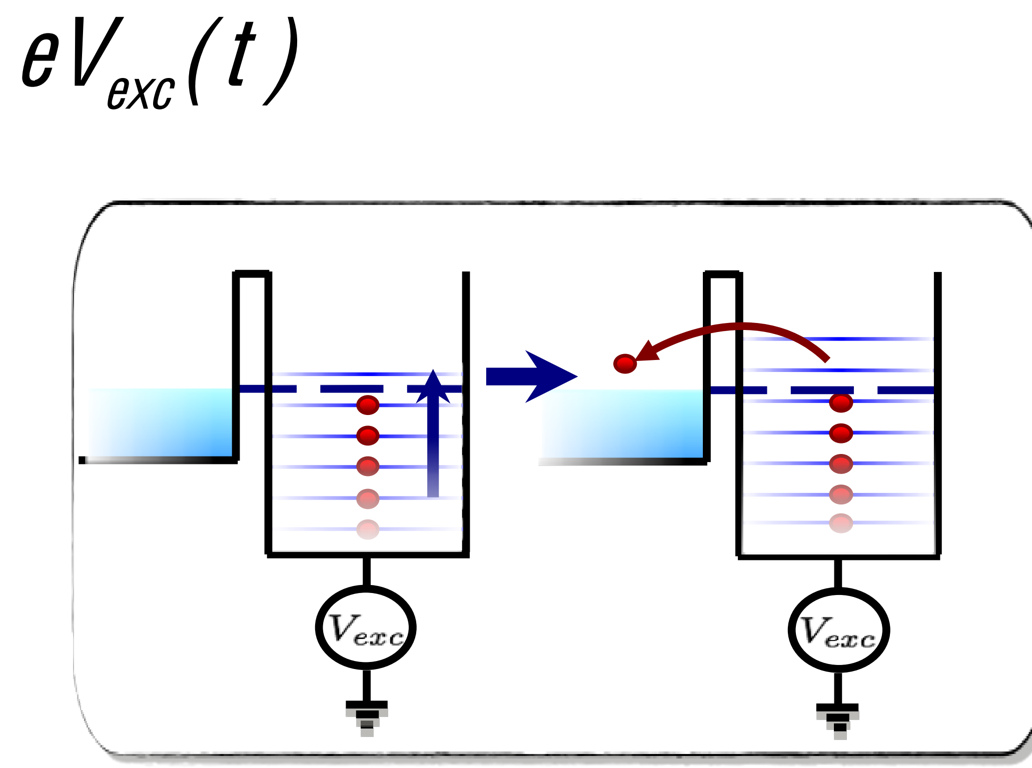
STRONG COUPLING QUANTUM THERMODYNAMICS IN ADIABATICALLY DRIVEN ELECTRON SYSTEMS

Experimental motivation: Quantum capacitors and single-particle emiters





G. Fève et al., Science **316**, 1169 (2007)

RAPID COMMUNICATIONS

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

Dynamical energy transfer in ac-driven quantum systems

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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.

DOI: 10.1103/PhysRevB.89.161306 PACS number(s): 73.23.−b, 72.10.Bg, 73.63.Kv, 44.10.+i

TUNNELING HAMILTONIAN MODEL

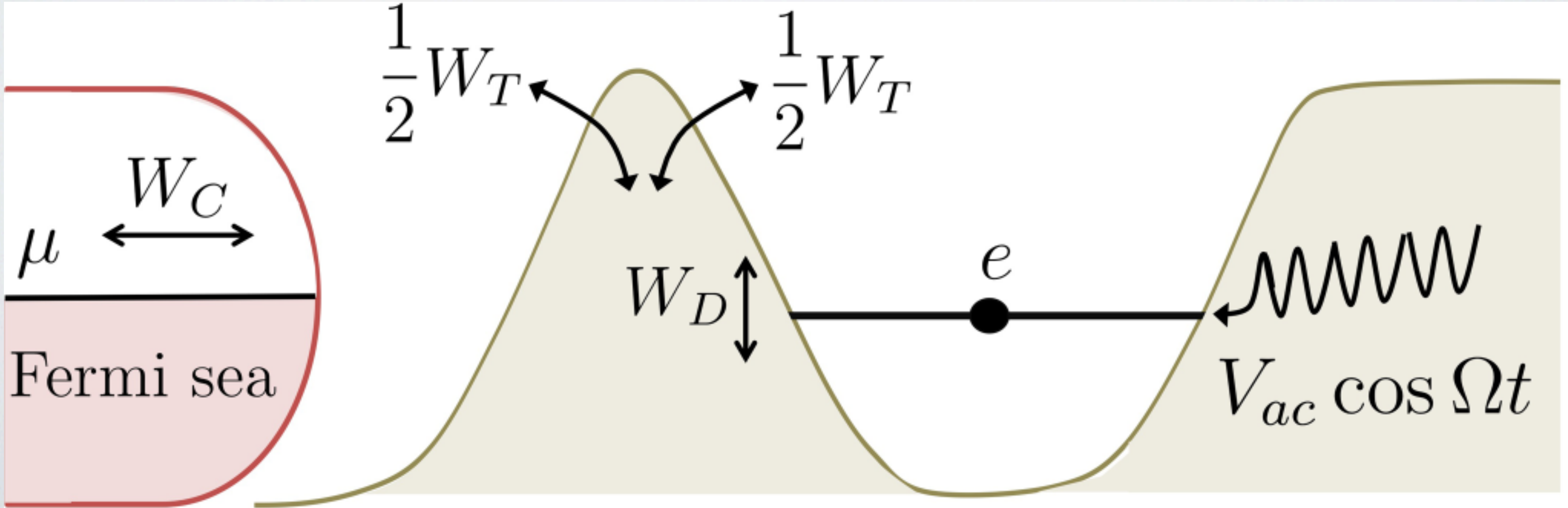
$\mathcal{H}_C = \sum_k \varepsilon_k c_k^\dagger c_k$

$\mathcal{H}_T = \sum_k (w_k d^\dagger c_k + \text{H.c.})$

$\mathcal{H}_D(t) = \varepsilon_d(t) d^\dagger d$

$\varepsilon_d(t) = \varepsilon_0 + V_{\text{ac}} \cos(\Omega t)$

$$\mathcal{H} = \mathcal{H}_C + \mathcal{H}_T + \mathcal{H}_D(t), \quad (1)$$



CHARGE AND ENERGY DYNAMICS

$$\frac{<d\mathcal{H}>}{dt} = W_C(t) + W_T(t) + W_D(t) + P(t)$$

$W_C(t) = \frac{i}{\hbar}\langle[\mathcal{H}, \mathcal{H}_C]\rangle,$

$W_T(t) = \frac{i}{\hbar}\langle[\mathcal{H}, \mathcal{H}_T]\rangle,$

$W_D(t) = \frac{i}{\hbar}\langle[\mathcal{H}, \mathcal{H}_D]\rangle,$

$P(t) = \langle\frac{\partial \mathcal{H}_D}{\partial t}\rangle$

$$W_C(t) + W_T(t) + W_D(t) = 0$$

$\overline{W_C} + \overline{W_D} = 0,$

$\overline{W_T} = 0,$ "Energy reactance"

$\overline{W_\alpha} = \frac{1}{\tau}\int_0^\tau dt W_\alpha(t), \quad \tau = \frac{2\pi}{\Omega}$

Charge conservation:

$$I_C(t) + I_D(t) = \overline{I_C} + \overline{I_D} = 0$$

EXACT EVALUATION OF FLUXES

I. Scattering Matrix (also referred to a Landauer-Büttiker)

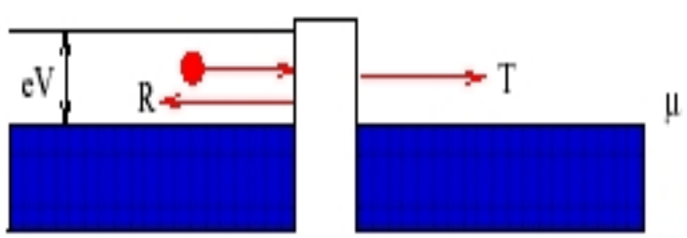
A. Stationary case:

Lectures by Markus Büttiker http://www.ffn.ub.es/~oleg/buttiker/scattering-theory.htm

Conductance from transmission

5

Heuristic discussion



Fermi energy left contact $\mu + eV$

Fermi energy right contact μ ,

applied voltage eV ,

transmission probability T ,

reflection probability R ,

incident current $I_{in} = ev_F \Delta\rho$

density $\Delta\rho = (d\rho/dE)\, eV$

density of states $d\rho/dE = (d\rho/dk)\,(dk/dE) = (1/2\pi)\,(1/\hbar v_F)$

$\Rightarrow$ $I_{in} = (e/h)eV$ independent of material !!

$I = (e/h)TeV \Rightarrow$

$$G = dI/dV = \frac{e^2}{h}T$$

Scattering matrix

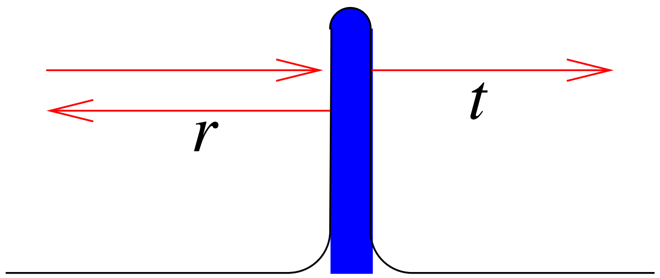
7

scattering state

$|\Psi>_{inc} = e^{ikx}$

$|\Psi>_{ref} = re^{-ikx}$

$|\Psi>_{tra} = t\, e^{ikx}$



scattering matrix

$$\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

current conservation $\Rightarrow$ S is a unitray matrix

In the absence of a magnetic field S is an orthogonal matrix

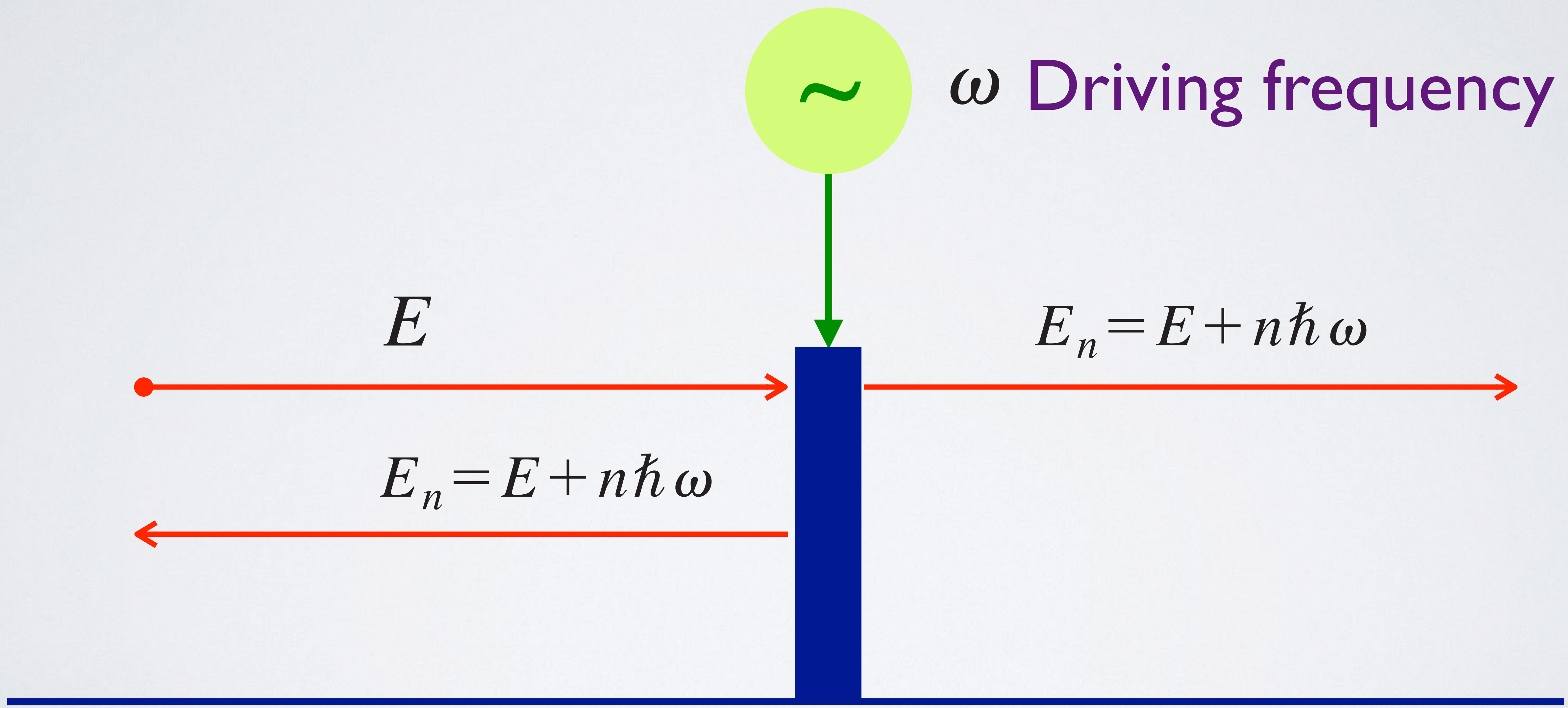
$t' = t$

I. Scattering Matrix (SM)

PHYSICAL REVIEW B **66**, 205320 (2002)

B. Time-periodic case: **Floquet scattering theory of quantum pumps**

M. Moskalets[1] and M. Büttiker[2]
[1]*Department of Metal and Semiconductor Physics, National Technical University "Kharkov Polytechnical Institute," Kharkov, Ukraine*
[2]*Département de Physique Théorique, Université de Genève, CH-1211 Genève 4, Switzerland*
(Received 19 August 2002; published 26 November 2002)



Outgoing $$\hat{b}_\alpha(E) = \sum_\beta \sum_{E_n>0} S_{F,\alpha\beta}(E,E_n)\hat{a}_\beta(E_n)$$ Incoming

II. Baym-Kadanoff-Schwinger-Keldysh non-equilibrium Green's functions (GF)

H Haug and AP Jauho, Springer Solid-State Sciences 123 (1996)
A. Kamenev Les Houches notes: cond-mat/0412296
J. Rammer, Cambridge University Press (2007)
R. Van Leeuwen, N. E. Dahlen, G. Stefanucci, C.O.Almblach, U.Von Barth, Lecture notes in Physics (chapter) Springer (2006)

$$H = h + H'(t) \; .$$

Switched on at t_0

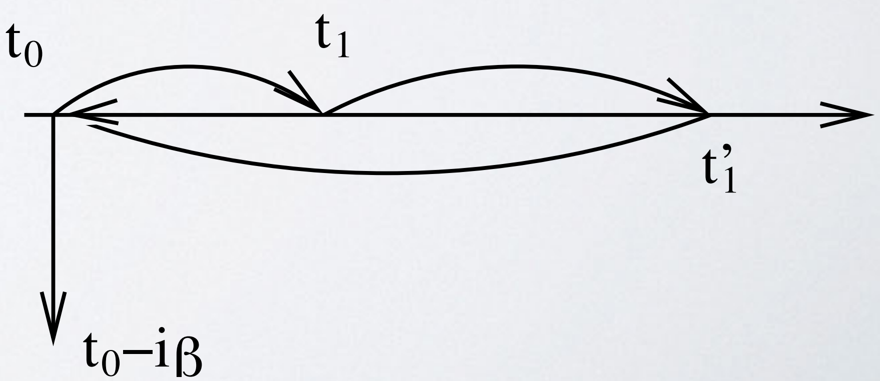
Before t_0

$$\varrho(h) = \frac{\exp(-\beta h)}{\mathrm{Tr}[\exp(-\beta h)]} \; .$$

Goal: evaluation of t-dependent values of observables

$$\langle O(t) \rangle = \mathrm{Tr}[\varrho(h) O_H(t)] \; .$$

$$G(1,1') \;\equiv\; -i\langle T_{C_v}[\psi_H(1)\psi_H^\dagger(1')]\rangle \; ,$$



II. Non-equilibrium Green's functions (GF) in systems with periodic driving

Floquet GF + master equations

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Available online at www.sciencedirect.com

SCIENCE DIRECT

Physics Reports 395 (2004) 1–157

PHYSICS REPORTS

www.elsevier.com/locate/physrep

Photon-assisted transport in semiconductor nanostructures

Gloria Platero*, Ramón Aguado

ELSEVIER

Available online at www.sciencedirect.com

SCIENCE DIRECT

Physics Reports 406 (2005) 379–443

PHYSICS REPORTS

www.elsevier.com/locate/physrep

Driven quantum transport on the nanoscale

Sigmund Kohler*, Jörg Lehmann[1], Peter Hänggi

Keldysh formalism in Floquet representation

PHYSICAL REVIEW B **72**, 125349 (2005)

Green-function approach to transport phenomena in quantum pumps

Liliana Arrachea

PHYSICAL REVIEW B **75**, 035319 (2007)

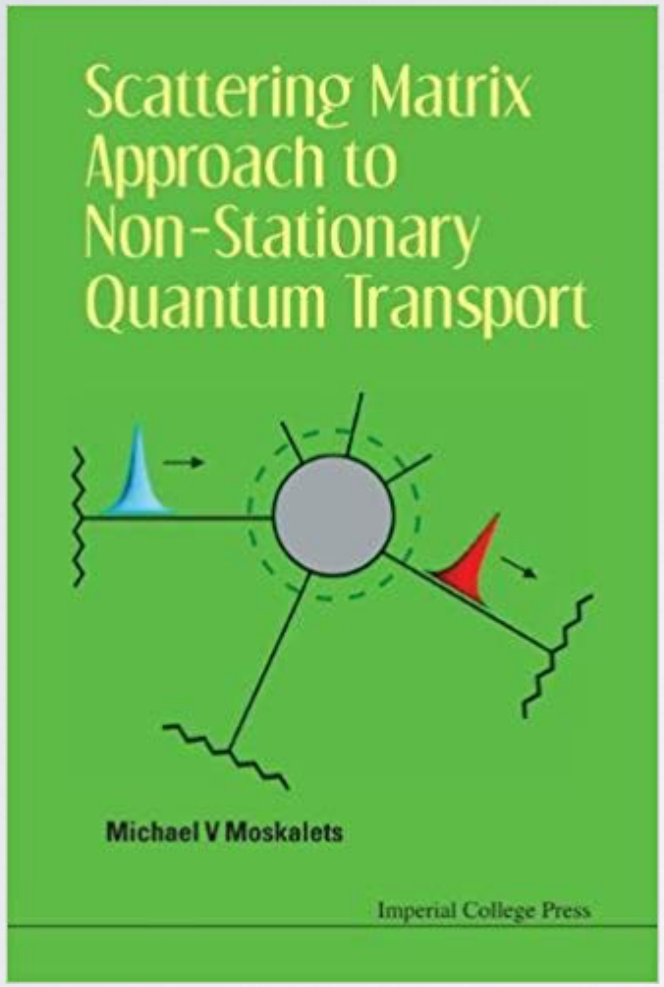
Exact Green's function renormalization approach to spectral properties of open quantum systems driven by harmonically time-dependent fields

Liliana Arrachea

$$G^R_{l,l'}(t,t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} G^R_{l,l'}(t,\omega),$$

$$\hat{G}^R(t,\omega) = \sum_{k=-\infty}^{\infty} \hat{\mathcal{G}}(k,\omega) e^{-ik\Omega_0 t},$$

SCHWINGER-KELDYSH GREEN'S FUNCTIONS AND SCATTERING MATRIX



Keldysh Green function: Evaluates time-dependent mean values of any observable in a non-equilibrium system. In particular:

$W_C(t)$ $W_T(t)$ $W_D(t)$

In addition: $P(t)$ $n_d(t)$ $\cdots$ etc

No discrimination of system and coupling. Evaluates fluxes in reservoirs.

RELATION BETWEEN SM AND GF

Stationary dc transport: Fisher and Lee, PRB 23, 6851 (1981)

PHYSICAL REVIEW B **74**, 245322 (2006)

Relation between scattering-matrix and Keldysh formalisms for quantum transport driven by time-periodic fields

Liliana Arrachea[1,2] and Michael Moskalets[3]

$$S^F(\varepsilon_m, \varepsilon_n) = \delta_{m,n} - i\Gamma \mathcal{G}^r(m-n, \varepsilon_n)$$

$$\Gamma = 2\pi \sum_k |w_k|^2 \delta(\varepsilon - \varepsilon_k)$$

Floquet Scattering Matrix

$$\mathcal{G}^r(t, \varepsilon) = \sum_n e^{-in\Omega t} \mathcal{G}(n, \varepsilon)$$

Steady state or t-dependent averages in ac driving:

Fluxes evaluated with SM coincide with fluxes in the reservoirs evaluated with GF.

SCATTERING MATRIX APPROACH

Model Hamiltonian in 1st quantization

$$\mathcal{H} = -\hbar^2\nabla^2/2m + U(t,\vec{r})$$

Continuity equation

$$\partial_t \rho_E + \nabla \cdot W_E = S_E,$$

$$\rho_E = \Psi^* \mathcal{H} \Psi$$

$$W_E = (\hbar/4mi)[\Psi^* \mathcal{H} \nabla \Psi - \nabla \Psi^* \mathcal{H} \Psi + \text{h.c.}]$$

$$S_E = \Psi^* \partial_t U \Psi$$

Energy flux to the reservoir

$$W_E(t) = \sum_{n,q} e^{-in\Omega t} \int d\varepsilon \frac{\varepsilon_q + \varepsilon_{n+q}}{2h} S^{F*}(\varepsilon_q, \varepsilon) S^F(\varepsilon_{n+q}, \varepsilon)[f(\varepsilon_q) - f(\varepsilon)]$$

ENERGY FLUXES. SCHWINGER-KELDYSH FORMALISM

Energy fluxes

$$W_C = -\frac{2}{\hbar}\mathrm{Re}\{\int dt_1 \int \frac{d\varepsilon}{2\pi}\, e^{-i\varepsilon(t_1-t)/\hbar}\left[i\mathcal{G}^r(t,t_1)\Gamma f(\varepsilon)\varepsilon + \int \frac{d\varepsilon'}{2\pi}\mathcal{G}^<(t,t_1)\Gamma\frac{\varepsilon'}{\varepsilon-\varepsilon'-i\eta}\right]\}$$

$$W_T(t) = 2\mathrm{Re}\{\int \frac{d\varepsilon}{h}\partial_t\mathcal{G}^r(t,\varepsilon)\Gamma f(\varepsilon)\}.$$

$$W_D = -\varepsilon_d(t)I_C(t)/e.$$

Charge current

$$I_C(t) = \frac{e}{h}\mathrm{Im}\{\int d\varepsilon\Gamma\left[2\mathcal{G}^r(t,\varepsilon)f(\varepsilon)+\mathcal{G}^<(t,\varepsilon)\right]\}.$$

Green functions

$$\mathcal{G}^r(t,t_1) = -i\theta(t-t_1)\langle\{d(t),d^\dagger(t_1)\}\rangle,$$
$$\mathcal{G}^<(t,t_1) = i\langle d^\dagger(t_1)d(t)\rangle,$$

$$\mathcal{G}(t,t_1) = \int \frac{d\varepsilon}{2\pi}e^{-i\varepsilon(t-t_1)/\hbar}\mathcal{G}(t,\varepsilon),$$

GREEN'S FUNCTION VS SCATTERING MATRIX IN TIME-DEPENDENT SYSTEMS

Different results in the time-dependent case!?

Energy flux in continuum

Energy reactance

Energy flux in reservoir

$$W_E(t) = W_C(t) + \frac{1}{2} W_T(t)$$

HOW TO DEFINE THE HEAT CURRENT FLOWING INTO THE RESERVOIR IN THE TIME DOMAIN?

$$\dot{\tilde{Q}}(t) = W_C(t) - \mu I_C(t)/e.$$

Without ER, not equal SM

?

or:

$$\dot{Q}(t) = W_E(t) - \mu I_C(t)/e$$

With ER, equal SM

$$W_E(t) = W_C(t) + \frac{1}{2} W_T(t)$$

FOCUS ON ADIABATIC REGIME

Period of driving fields much larger than any characteristic time for the electrons in the quantum dot

$$\tau = \frac{2\pi}{\Omega} \gg t_e \sim \frac{h}{\Gamma}$$

The energy $\hbar\Omega$ is the lowest energy scale of the system

CHECKING THE SECOND LAW

Slow driving regime: adiabatic expansion in powers of Ω

$$\mathcal{G}^r(t,\varepsilon) = \mathcal{G}_f^r(t,\varepsilon) + \frac{i\hbar}{2}\partial_t\partial_\varepsilon\mathcal{G}_f^r(t,\varepsilon) + \dots$$

$$\mathcal{G}_f^r(t,\varepsilon) = [\varepsilon - \varepsilon_d(t) + i\Gamma/2]^{-1}$$

Ω

Ω^2

$$\dot{Q}(t) = \dot{Q}^{(1)}(t) + \dot{Q}^{(2)}(t)$$

$T = 0$

Instantaneous Joule law

Agreement with 2nd law!

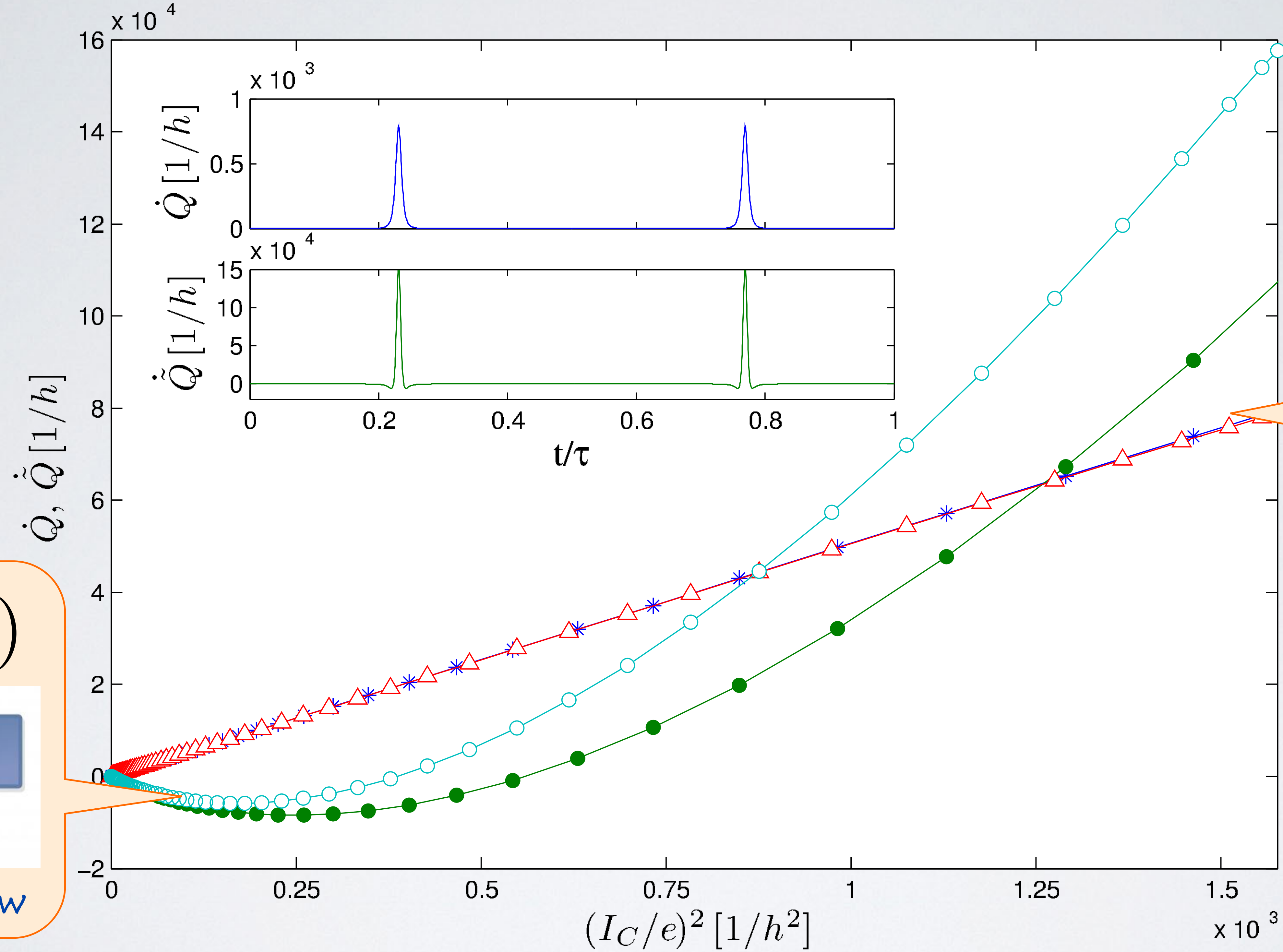
$$\dot{Q}^{(1)}(t) = 0$$

$$\dot{Q}^{(2)}(t) = R_q[I_C^{(1)}(t)]^2$$

Büttiker resistance

$R_q = h/2e^2$

T=0 → Heat must flow into the reservoir



$\dot{Q}(t)$

2nd law

$\dot{\tilde{Q}}(t)$

2nd law

However $\overline{\dot{\tilde{Q}}} = \overline{\dot{Q}}$ because $\overline{W_T} = 0$

SUMMARY (I)

I. The following definition of the **time-dependent heat current flowing into the reservoir**:

$$\dot{Q}(t) = W_C(t) + \frac{1}{2} W_T(t) - \mu I_C(t)/e$$

Can be expressed as instantaneous Joule law and recovers the results obtained with Scattering matrix.

II. Verified in:

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)

IV. No claims about reduced density matrix.

OTHER EFFECTS:

SEVERAL RESERVOIRS

FINITE TEMPERATURE

VOLTAGE BIAS

PHYSICAL REVIEW B **94**, 035436 (2016)

Dynamics of energy transport and entropy production in ac-driven quantum electron systems

María Florencia Ludovico,[1,2] Michael Moskalets,[3] David Sánchez,[4] and Liliana Arrachea[1,2]
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(Received 13 April 2016; revised manuscript received 21 June 2016; published 21 July 2016)

We analyze the time-resolved energy transport and the entropy production in ac-driven quantum coherent electron systems coupled to multiple reservoirs at finite temperature. At slow driving, we formulate the first and second laws of thermodynamics valid at each instant of time. We identify heat fluxes flowing through the different pieces of the device and emphasize the importance of the energy stored in the contact and central regions for the second law of thermodynamics to be instantaneously satisfied. In addition, we discuss conservative and dissipative contributions to the heat flux and to the entropy production as a function of time. We illustrate these ideas with a simple model corresponding to a driven level coupled to two reservoirs with different chemical potentials.

DOI: 10.1103/PhysRevB.94.035436

Review

Periodic Energy Transport and Entropy Production in Quantum Electronics

María Florencia Ludovico [1], Liliana Arrachea [1], Michael Moskalets [2] and David Sánchez [3,*]

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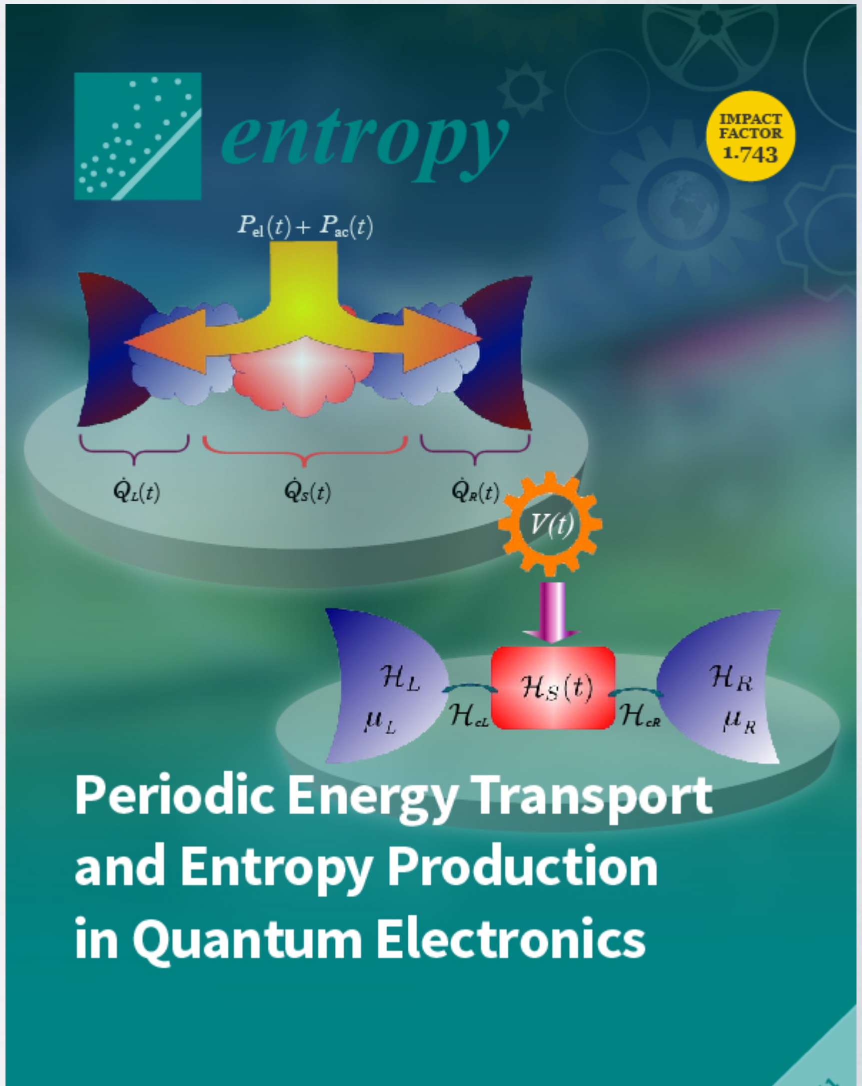
Academic Editor: Ronnie Kosloff
Received: 4 October 2016; Accepted: 15 November 2016; Published: 23 November 2016



MODEL

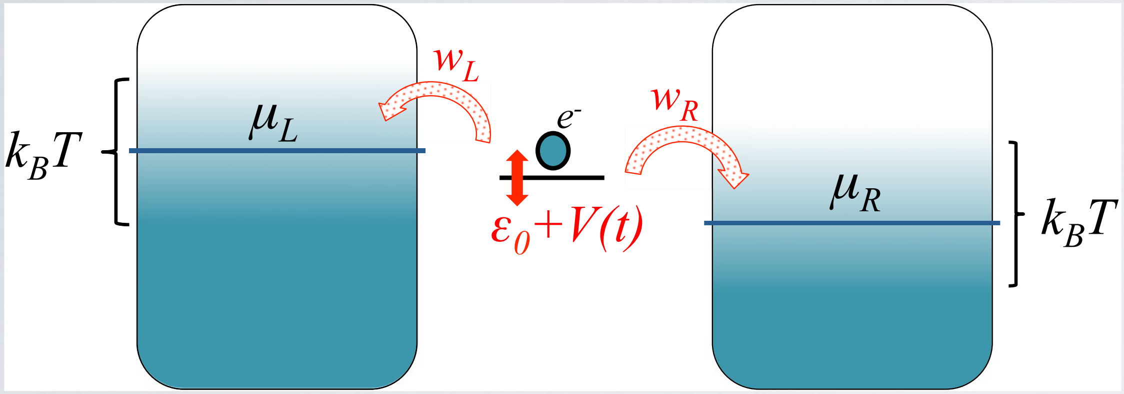


FIG. 1. A single electronic level is coupled to two reservoirs (fermionic baths) kept at the same temperature T. The chemical potentials of the left and right reservoirs are $\mu_L = \mu$ and $\mu_R = \mu - \delta\mu$, respectively. The electronic level slowly evolves in time with a periodic parameter $V(t)$, and hence after a completed period the central part of the systems returns to its initial state.

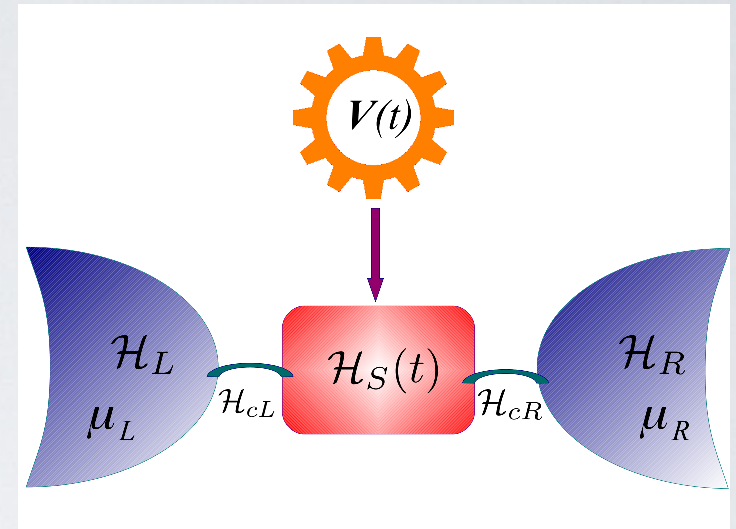


Figure 1. Sketch of the system under consideration. A quantum conductor (described by the Hamiltonian H_S), is coupled to two reservoirs (H_L and H_R) kept at the same temperature T, but with different chemical potentials μ_L and μ_R. The conductor is also driven out of equilibrium by the application of AC local power sources, which are all collected in the vector $\mathbf{V}(t)$. The Hamiltonians representing the left and right contact regions are H_{cL} and H_{cR}, respectively.

$$\mathcal{H}(t) = \mathcal{H}_{\text{res}} + \mathcal{H}_S(t) + \mathcal{H}_{\text{cont}}.$$

$$\mathcal{H}_{\text{res}} = \sum_\alpha \mathcal{H}_\alpha$$

$$\mathcal{H}_S(\mathbf{V}(t))$$

$$\mathcal{H}_{\text{cont}} = \sum_\alpha \mathcal{H}_{c\alpha}$$

$$\mathbf{V}(t) = \mathbf{V}(t+\tau) = (V_1(t), \ldots, V_M(t))$$

$$\mathcal{H}_{c\alpha} = \sum_{k_\alpha, l_\alpha} \left(w_{k_\alpha, l_\alpha} c^\dagger_{k_\alpha} d_{l_\alpha} + \text{H.c.} \right),$$

QUANTUM KINETICS OF CHARGE AND ENERGY

Conservation laws

$$e\langle\dot{\mathcal{N}}\rangle = I_S^C(t) + \sum_\alpha I_\alpha^C(t) = 0 \qquad (1)$$

Charge

$$I_\nu^C(t) = e\langle\dot{\mathcal{N}}_\nu\rangle = \frac{ie}{\hbar}\langle[\mathcal{H},\mathcal{N}_\nu]\rangle$$

$$\langle\dot{\mathcal{H}}\rangle = \sum_\alpha\left[J_\alpha^E(t) + J_{c\alpha}^E(t)\right] + J_S^E(t) - \mathbf{F}\cdot\dot{\mathbf{V}} \qquad (2)$$

Energy

$$J_\nu^E(t) = \frac{i}{\hbar}\langle[\mathcal{H},\mathcal{H}_\nu]\rangle$$

$$P_{\rm ac}(t) = \mathbf{F}\cdot\dot{\mathbf{V}}.$$

$$\mathbf{F} = -\left\langle\frac{\partial\mathcal{H}}{\partial\mathbf{V}}\right\rangle$$

$$\sum_\alpha\left[J_\alpha^E(t) + J_{c\alpha}^E(t)\right] + J_S^E(t) = 0$$

$$P_{\rm ac}(t) = -\langle\dot{\mathcal{H}}\rangle$$

Eq.(2) -μ/e Eq. (1):

$$\sum_\alpha \left[J_\alpha^E(t) - \mu_\alpha \frac{I_\alpha^C(t)}{e} + J_{c\alpha}^E(t) \right] + J_S^E(t) - \mu \frac{I_S^C(t)}{e} + P_{\rm el}(t) = 0$$

$$P_{\rm el}(t) = \sum_\alpha \frac{I_\alpha^C(t)}{e} \delta\mu_\alpha$$

$$\mu_\alpha = \mu + \delta\mu_\alpha$$

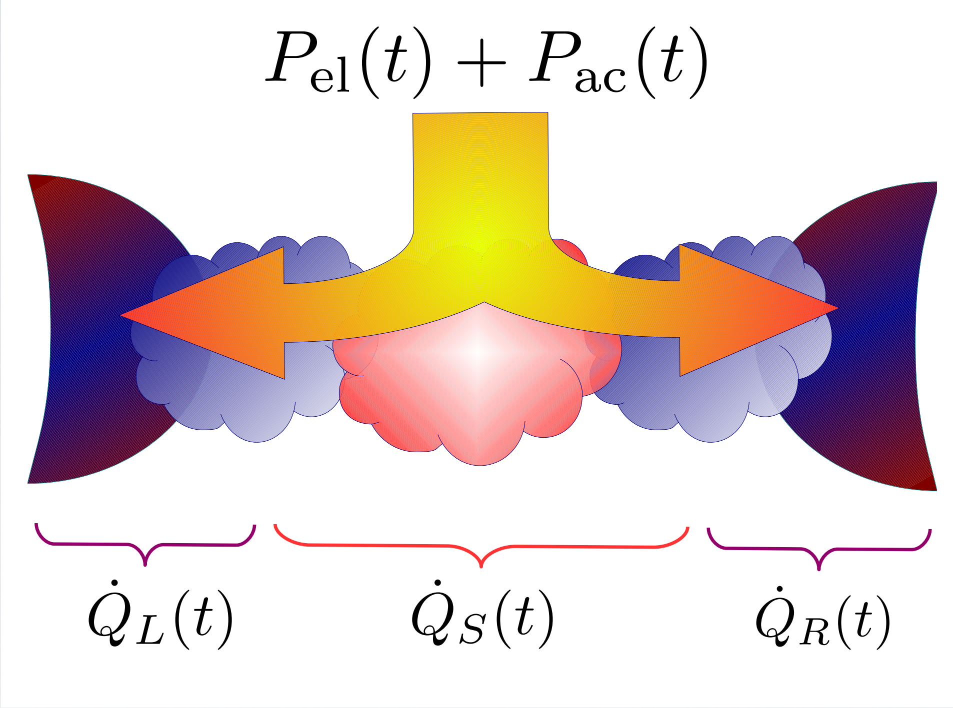
Subtract in both terms $P_{\rm ac}(t)$.

$$\sum_\alpha \left[J_\alpha^E(t) - \mu_\alpha \frac{I_\alpha^C(t)}{e} + J_{c\alpha}^E(t) \right] + J_S^E(t) - \mu \frac{I_S^C(t)}{e} - P_{\rm ac}(t) = -P_{\rm ac}(t) - P_{\rm el}(t).$$

$\dot{Q}_{\rm tot}(t)$ Heat

Power

Distribution of the total heat (interpretation)



$$\dot{Q}_{\rm tot}(t) = \sum_\alpha \left[J^E_\alpha(t) - \mu_\alpha \frac{I^C_\alpha(t)}{e} + J^E_{c\alpha}(t) \right] + J^E_S(t) - \mu \frac{I^C_S(t)}{e} - P_{\rm ac}(t)$$

$$\dot{Q}_\alpha(t) = J^E_\alpha(t) + \frac{J^E_{c\alpha}(t)}{2} - \mu_\alpha \frac{I^C_\alpha(t)}{e}.$$

Energy reactance

$$\dot{Q}_S(t) = \dot{E}_S(t) - \mu \frac{I^C_S(t)}{e} + \sum_\alpha \frac{J^E_{c\alpha}(t)}{2}.$$

$$\dot{E}_S(t) \equiv \langle \dot{\mathcal{H}}_S \rangle = J^E_S(t) - P_{\rm ac}(t)$$

$$\dot{Q}_{\rm tot}(t) = \sum_\alpha \dot{Q}_\alpha(t) + \dot{Q}_S(t).$$

ENTROPY PRODUCTION

$$\dot{Q}_{\text{tot}}(t) = \sum_{\alpha} \dot{Q}_{\alpha}(t) + \dot{Q}_S(t).$$

$$\dot{Q}_{\alpha}(t) = J^E_{\alpha}(t) + \frac{J^E_{c\alpha}(t)}{2} - \mu_{\alpha}\frac{I^C_{\alpha}(t)}{e}.$$

$$\dot{Q}_S(t) = J^E_S(t) - P_{\text{ac}}(t) - \mu\frac{I^C_S(t)}{e} + \sum_{\alpha}\frac{J^E_{c\alpha}(t)}{2}$$

$$\dot{S}_{\text{tot}} = \dot{S}^{\text{cons}}(t) + \dot{S}^{\text{non cons}}(t) \quad \begin{cases} \dot{S}^{\text{cons}}(t) = \dfrac{1}{T}\dot{Q}^{\text{cons}}(t) = -\dfrac{1}{T}P^{\text{cons}}(t) \\ \dot{S}^{\text{non cons}}(t) = \dfrac{1}{T}\dot{Q}^{\text{non cons}}_{\text{tot}}(t) \end{cases}$$

$$\dot{Q}^{\text{non cons}}_{\text{tot}}(t) = \sum_{\alpha}\dot{Q}_{\alpha}(t) + \dot{Q}^{\text{non cons}}_S(t)$$

$$\dot{Q}^{\text{non cons}}_S(t) = \dot{Q}_S(t) + P^{\text{cons}}_{\text{tot}}(t)$$

NET CONTRIBUTIONS

$$\sum_\alpha \overline{J_\alpha^E} = -\overline{J_S^E} = -\overline{P_{\rm ac}}, \quad \sum_\alpha \overline{I_\alpha^C} = 0,$$

$$\overline{J_{c\alpha}^E} = \overline{I_S^C} = 0,$$

$$\overline{\dot{Q}_{\rm tot}} = \sum_\alpha \overline{\dot{Q}_\alpha} = -\overline{P_{\rm ac}} - \overline{P_{\rm el}},$$

$$\overline{\dot{Q}_\alpha} = \overline{J_\alpha^E} - \mu_\alpha \frac{\overline{I_\alpha^C}}{e}$$

The energy reactance does not contribute to the net rate of heat production. It is a purely time-dependent effect

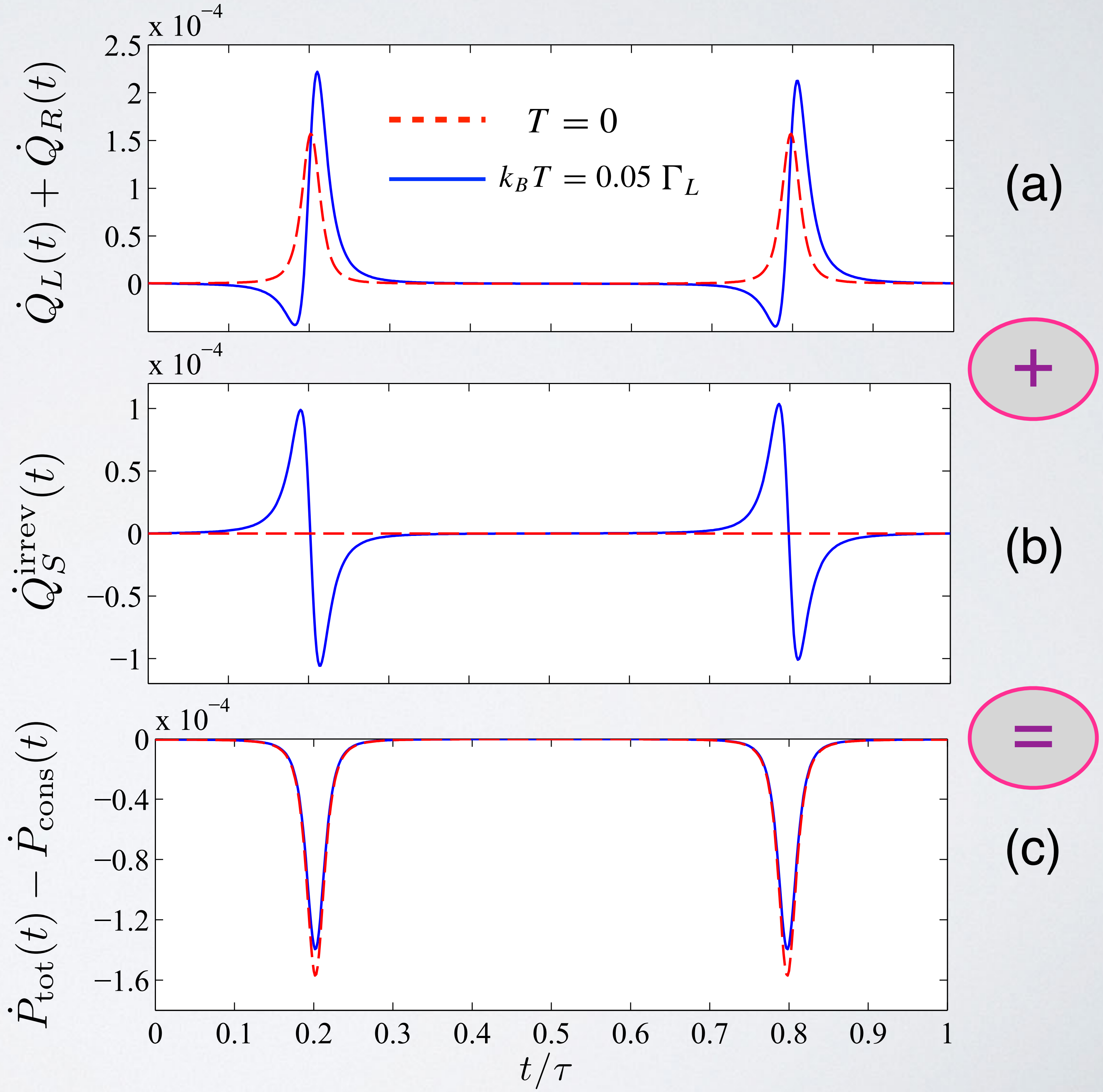
EXAMPLE: ADIABATIC REGIME

$$\mathcal{H}_S = \varepsilon_d(t) d^\dagger d, \quad \varepsilon_d(t) = \varepsilon_0 + V_0 \cos(\omega t) \quad \mu_L = \mu \quad \mu_R = \mu - \delta\mu$$

Total heat flux in reservoirs with energy reactance.
Exact results with SM = GF

Non-conservative heat flux in system
Exact results with GF

Non-conservative Power by external forces
Exact results with GF



SM=GF FOR HEAT CURRENT AT RESERVOIRS EVALUATED WITH ENERGY REACTANCE

$$\dot{Q}_\alpha(t) = J^E_\alpha(t) + \frac{J^E_{c\alpha}(t)}{2} - \mu_\alpha \frac{I^C_\alpha(t)}{e}.$$

Fermi function

GF

$$= \sum_l \int \frac{d\varepsilon}{h} e^{-il\omega t}\Gamma_\alpha \Big\{ i\mathcal{G}^*_{l_\alpha,l_\alpha}(-l,\varepsilon)(\varepsilon - \frac{l\hbar\omega}{2} - \mu_\alpha)(f_\alpha(\varepsilon) - f_\alpha(\varepsilon - l\hbar\omega))$$
$$- \sum_n \sum_{\beta=L,R} (\varepsilon + \frac{l\hbar\omega}{2} - \mu_\alpha)(f_\alpha(\varepsilon)-f_\beta(\varepsilon-n\hbar\omega))\Gamma_\beta \mathcal{G}_{l_\alpha,l_\beta}(l+n,\varepsilon-n\hbar\omega)\mathcal{G}^*_{l_\alpha,l_\beta}(n,\varepsilon-n\hbar\omega)\Big\}$$

SM

$$\dot{Q}_\alpha(t) = \sum_{l,n} e^{-il\omega t}\int\frac{d\varepsilon}{h}(\varepsilon+\frac{l\hbar\omega}{2}-\mu_\alpha)\sum_{\beta=L,R}(f_\beta(\varepsilon_{-n}) - f_\alpha(\varepsilon))S^*_{\alpha\beta}(\varepsilon,\varepsilon_{-n})S_{\alpha,\beta}(\varepsilon_l,\varepsilon_{-n}),$$

Replace: $S_{\alpha\beta}(\varepsilon_m,\varepsilon_n) = \delta_{\alpha,\beta}\delta_{m,n} - i\sqrt{\Gamma_\alpha(\varepsilon_m)\Gamma_\beta(\varepsilon_n)}\mathcal{G}_{l_\alpha,l_\beta}(m-n,\varepsilon_n).$

Get:

$$\sum_{l,n}\int\frac{d\varepsilon}{h}e^{-il\omega t}(\varepsilon+\frac{l\hbar\omega}{2}-\mu_\alpha)\sum_{\beta=L,R}(f_\beta(\varepsilon-n\hbar\omega)-f_\alpha(\varepsilon))\,\mathcal{G}^*_{l_\alpha,l_\beta}(n,\varepsilon-n\hbar\omega)\Big\{i\delta_{\alpha\beta}\delta_{l,-n}\sqrt{\Gamma_\alpha\Gamma_\beta}+\Gamma_\alpha\Gamma_\beta\mathcal{G}_{l_\alpha,l_\beta}(l+n,\varepsilon-n\hbar\omega)\Big\}$$

$$\ldots\ldots\ldots\ldots\ldots = \dot{Q}_\alpha(t)$$

SUMMARY (II)

I. The following definition of the **time-dependent heat current flowing into the reservoir**:

$$\dot{Q}_\alpha(t) = J^E_\alpha(t) + \frac{J^E_{c\alpha}(t)}{2} - \mu_\alpha \frac{I^C_\alpha(t)}{e}.$$

Can be expressed as instantaneous Joule law and recovers the results obtained with Scattering matrix in systems at any temperature, several reservoirs and finite applied voltages .

II. At finite temperatures: $\dot{Q}_{\rm tot}(t) = \sum_\alpha \dot{Q}_\alpha(t) + \dot{Q}_S(t).$

$$\dot{Q}^{irrev}_{\rm tot}(t) = -P^{\rm non\ cons}_{tot}(t)$$

COMMENT

In order to simplify calculations, a featureless density of states for the reservoirs was assumed: $\Gamma_\alpha(\varepsilon) \sim \Gamma$

Γ sets the typical time scale for the electrons in the quantum dot.

Adiabatic regime implies $\Gamma >> \hbar\omega$

Featureless $\Gamma_\alpha(\varepsilon) \sim \Gamma$ is a very reasonable assumption for the adiabatic regime at low T.

EXPERIMENTAL CONSEQUENCES OF THE ENERGY REACTANCE?

PHYSICAL REVIEW B **97**, 041416(R) (2018)

Rapid Communications

Probing the energy reactance with adiabatically driven quantum dots

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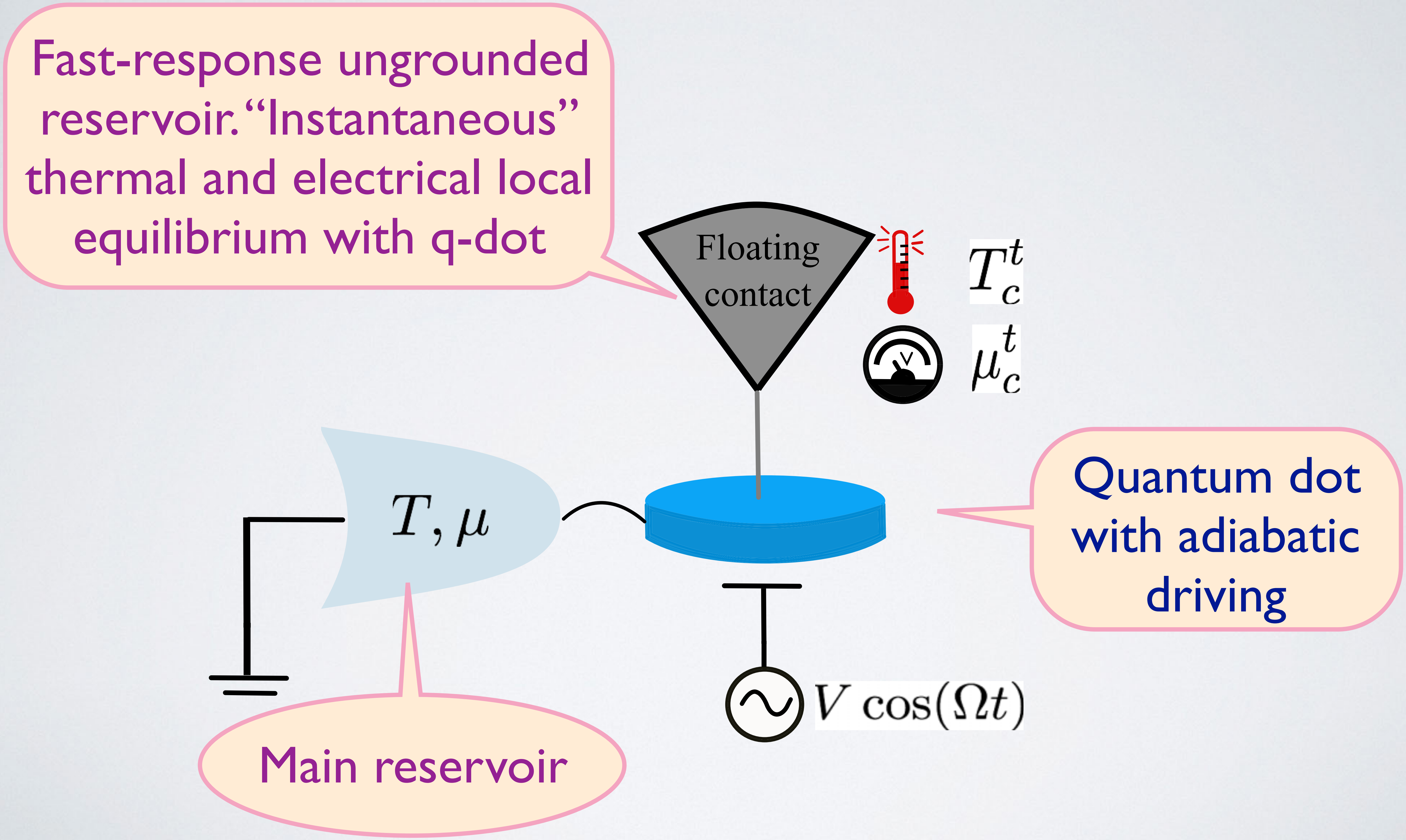
The tunneling Hamiltonian describes a particle transfer from one region to another. Although there is no particle storage in the tunneling region itself, it has an associated amount of energy. The corresponding energy flux was named reactance since, such as an electrical reactance, it manifests itself in time-dependent transport only. We show here that the existence of the *energy reactance* leads to the universal response of a mesoscopic thermometer, a floating contact coupled to an adiabatically driven quantum dot.

PROPOSED SETUP



THERMOELECTRIC DYNAMICS OF THE PROBE

$$\mathbf{J}(t) \equiv (\dot{N}_c, \dot{Q}_c) \qquad \mathbf{X}^t = (\delta\mu_c^t, \delta T_c^t, \hbar\Omega)$$

Assumptions:

*Linear response (small driving frequency)

*Fast response of the probe: chemical potential and temperature adapt immediately to nullify charge and heat current.

$$J_i(t) = \sum_{j=1}^{3} \Lambda_{ij}(t) X_j^t = 0 \qquad i = 1,2$$

RESULTS

Solution:

$$\sum_{j=1}^{2} \Lambda_{ij} X_j^t = -\Lambda_{i3}\hbar\Omega, \; i = 1,2.$$

$$\delta\mu_c^t = \frac{\Lambda_{12}\Lambda_{23} - \Lambda_{13}\Lambda_{22}}{\det \Lambda'}\hbar\Omega,$$

$$\delta T_c^t = \frac{\Lambda_{13}\Lambda_{21} - \Lambda_{11}\Lambda_{23}}{\det \Lambda'}\hbar\Omega,$$

Outcome depends on the adopted definition of the t-dependent heat current flowing into the probe.

RESULTS

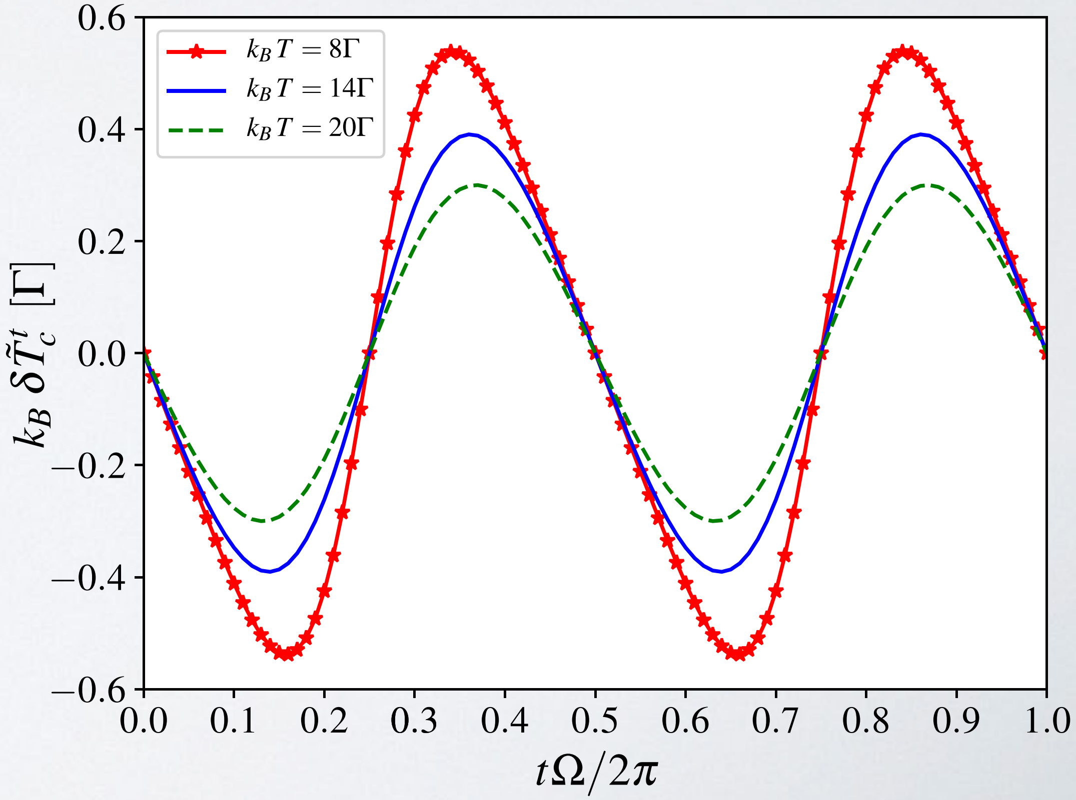
(a) Taking into account the energy reactance:

$$\dot{Q}_c(t) = \dot{U}_c(t) + \frac{\dot{U}_{T_c}(t)}{2} - \mu_c^t \dot{N}_c(t).$$

$$T_c^t = T,$$

(b) Without taking into account the energy reactance

$$\dot{\tilde{Q}}_c(t) = \dot{U}_c(t) - \mu_c^t \dot{N}_c(t).$$



SUMMARY (III)

The energy reactance could be tested by sensing the temperature of the probe.

FORCES AND POWER IN THE ADIABATIC REGIME

PHYSICAL REVIEW B **93**, 075136 (2016)

Adiabatic response and quantum thermoelectrics for ac-driven quantum systems

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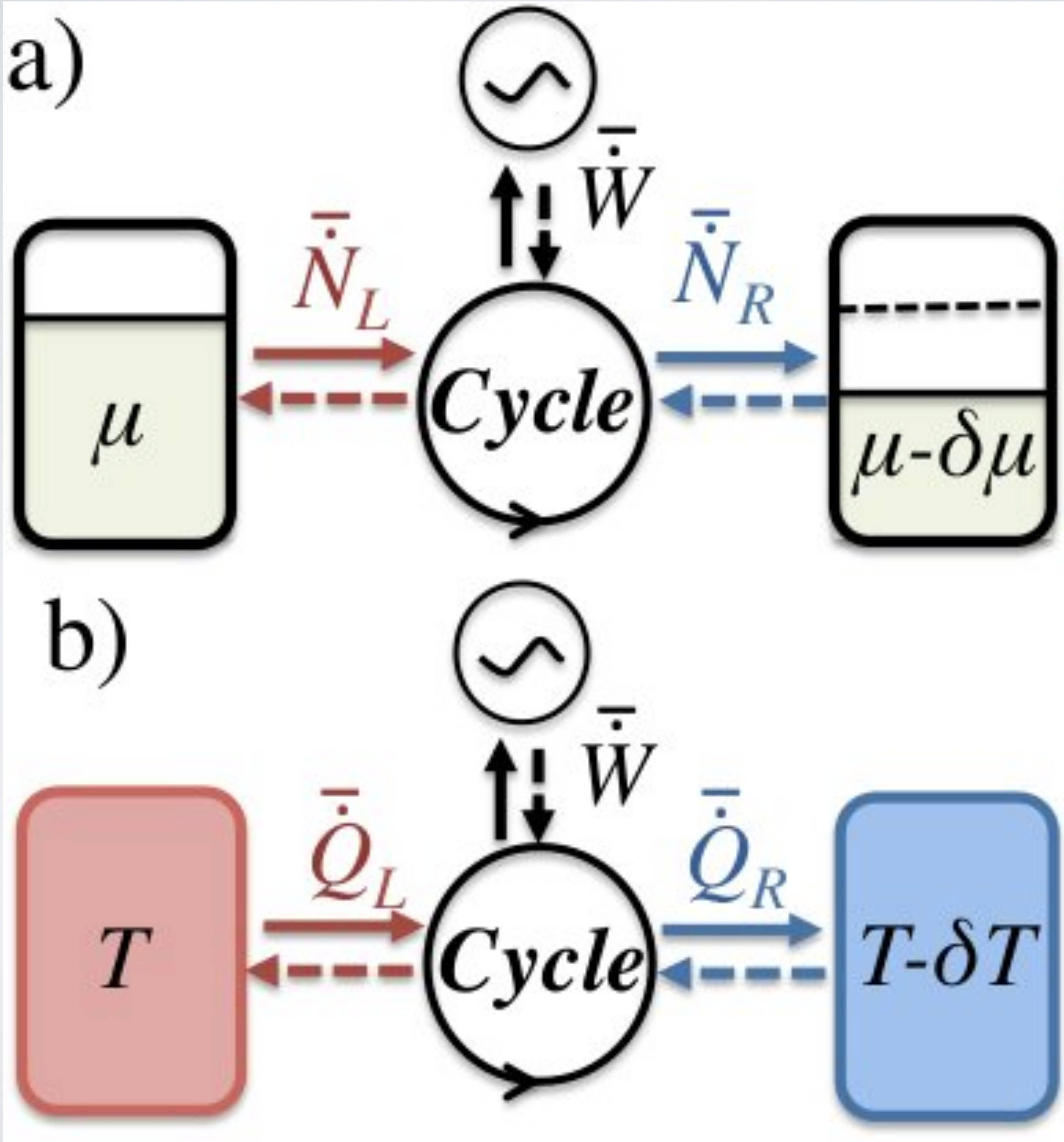
We generalize the theory of thermoelectrics to include coherent electron systems under adiabatic ac driving, accounting for quantum pumping of charge and heat, as well as for the work exchanged between the electron system and driving potentials. We derive the relevant response coefficients in the adiabatic regime and show that they obey generalized Onsager reciprocity relations. We analyze the consequences of our generalized thermoelectric framework for quantum motors, generators, heat engines, and heat pumps, characterizing them in terms of efficiencies and figures of merit. We illustrate these concepts in a model for a quantum pump.

DOI: 10.1103/PhysRevB.93.075136


a)
$\bar{\dot{W}}$
$\bar{\dot{N}}_L$
$\bar{\dot{N}}_R$
μ
Cycle
μ-$\delta\mu$
b)
$\bar{\dot{W}}$
$\bar{\dot{Q}}_L$
$\bar{\dot{Q}}_R$
T
Cycle
T-δT

ADIABATIC RESPONSE

Time-periodic Hamiltonian with $\mathcal{T} = 2\pi/\omega$

$$\mathcal{H} = \mathcal{H}(\mathbf{V}(t)) \qquad \mathbf{V}(t) = \mathbf{V}(t+\mathcal{T}) = (V_1(t), V_2(t), \ldots)$$

Evolution operator for linear response in $\dot{\mathbf{V}}(t)$

$$\hat{U}(t,t_0) \simeq \mathrm{T}\exp\{-i\hat{\mathcal{H}}_t(t-t_0) - i\int_{t_0}^{t} dt'(t-t')\hat{\mathbf{F}}\cdot\dot{\mathbf{V}}(t)\}$$

Force

$$\hat{\mathbf{F}}(t) = -\frac{\partial\hat{\mathcal{H}}(t)}{\partial\mathbf{V}(t)}$$

Generalized velocity

Mean value of an observable

$$O(t) \simeq \langle \hat{O} \rangle_t - i \int_{t_0}^{t} dt'(t-t')\langle \left[\hat{O}(t), \hat{\mathbf{F}}(t')\right] \rangle_t \dot{\mathbf{V}}(t)$$

$$= \langle \hat{O} \rangle_t + \mathbf{\Lambda}_t^{O\mathbf{F}} \cdot \dot{\mathbf{V}}(t).$$

Evaluated with frozen $\hat{\rho}_t$

Linear response coefficient:

$$\Lambda^{O\mathbf{F}} = \int_{-\infty}^{+\infty} d\tau \tau \chi_t^{O\mathbf{F}}(\tau) = \lim_{\Omega \to 0} \frac{\mathrm{Im}\left[\chi_t^{O\mathbf{F}}(\Omega)\right]}{\Omega}$$

Equilibrium (Kubo-like) susceptibility:

$$\chi_t^{O,\mathbf{F}}(t-t') = -i\theta(t-t')\langle [\hat{O}(t), \hat{\mathbf{F}}(t')] \rangle_t$$

Combining with usual Kubo treatment in $\delta\mu$

Conductance

Pumping

$$\begin{pmatrix} J^c(t) \\ \mathbf{F}(t) \end{pmatrix} = \begin{pmatrix} J^c_t \\ \mathbf{F}_t \end{pmatrix} + \begin{pmatrix} \Lambda^{cc}_t & \mathbf{\Lambda}^{cf}_t \\ \mathbf{\Lambda}^{fc}_t & \hat{\mathbf{\Lambda}}^{ff}_t \end{pmatrix} \begin{pmatrix} \delta\mu \\ \dot{\mathbf{V}}(t) \end{pmatrix}$$

Born-Oppenheimer

Non-conservative

Dissipation

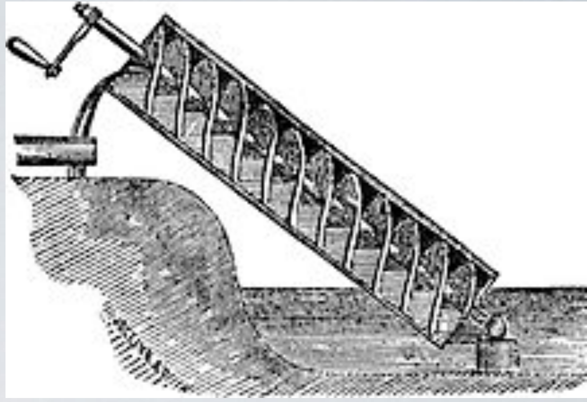
Onsager relations

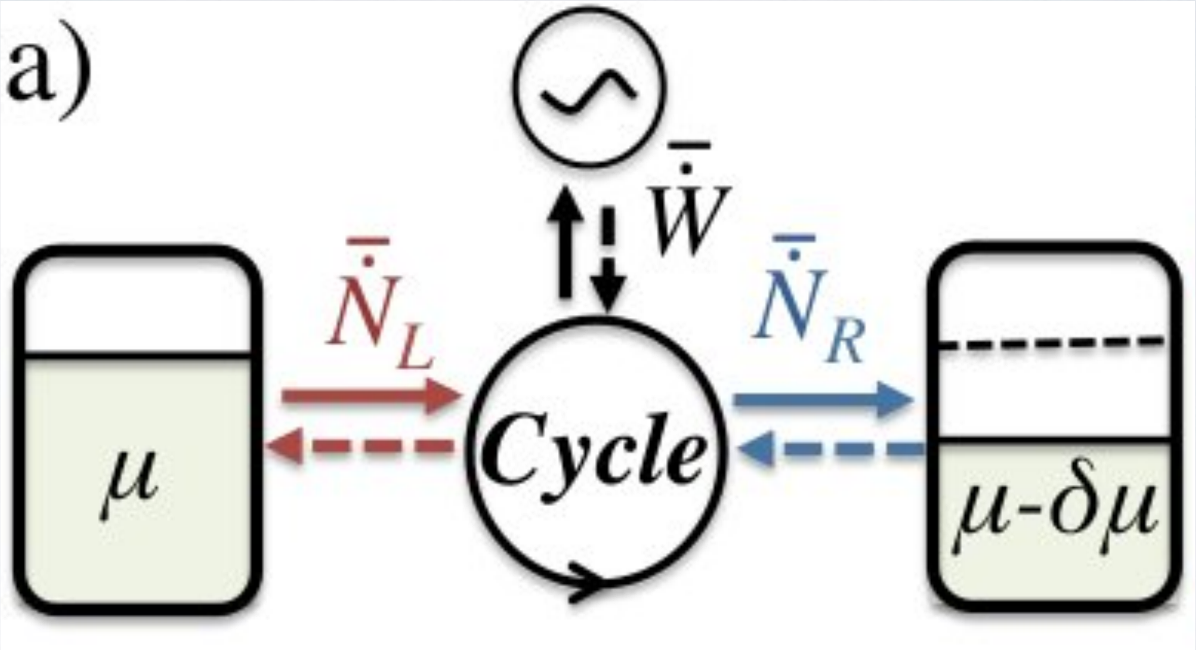
$$\Lambda^{cc}_t(B) = \Lambda^{cc}_t(-B) \quad , \quad \hat{\mathbf{\Lambda}}^{ff}_{ij}(B) = s_i s_j \hat{\mathbf{\Lambda}}^{ff}_{ji}(-B)$$

$$\mathbf{\Lambda}^{cf}_j(B) = s_j \mathbf{\Lambda}^{fc}_j(-B),$$

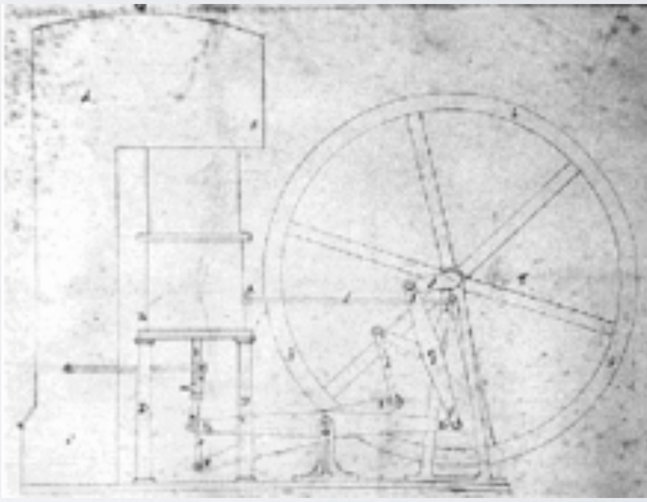
$s_j = \pm 1$ depending on parity under t-reversal

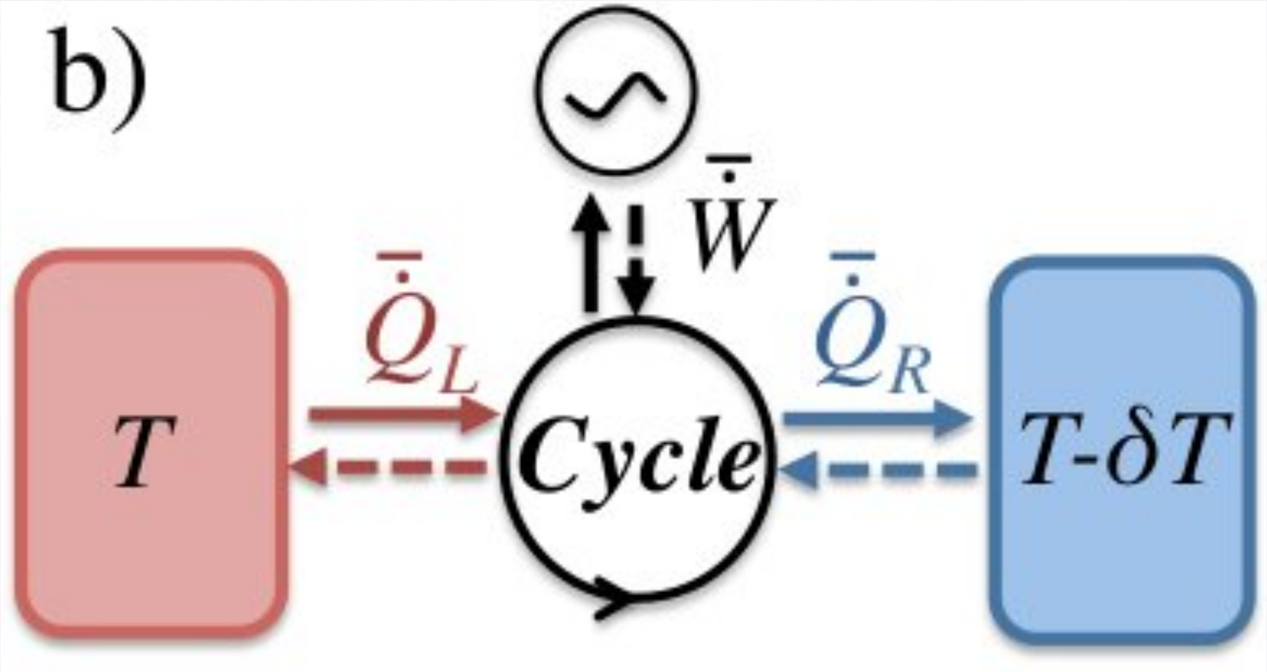
MOTORS/GENERATORS





HEAT PUMPS/HEAT ENGINES





PHYSICAL REVIEW B **95**, 235117 (2017)

Nonlinear charge and energy dynamics of an adiabatically driven interacting quantum dot

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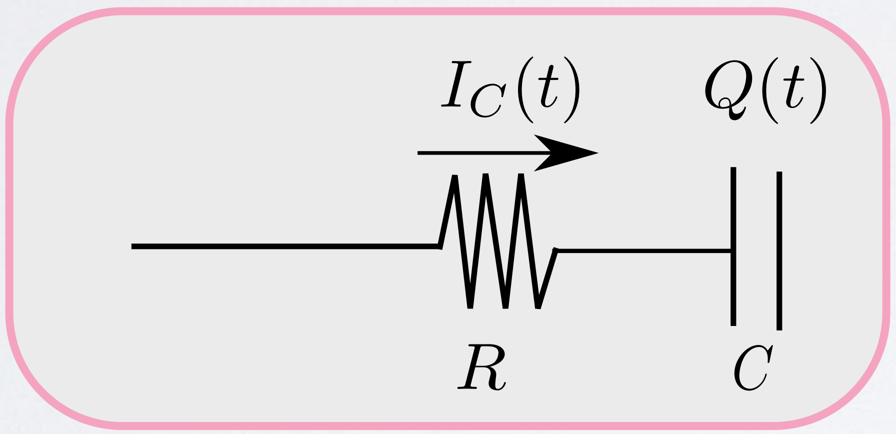
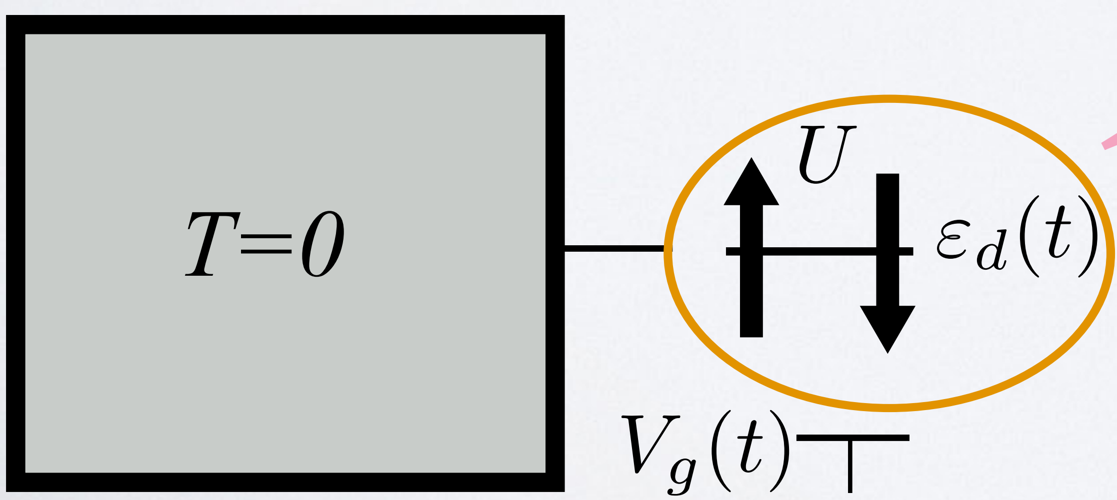
(Received 6 October 2016; revised manuscript received 12 May 2017; published 8 June 2017)

Adiabatic Kubo formalism + Numerical renormalization group



Coulomb interaction

$$H_{\rm dot}(t) = \sum_\sigma \varepsilon_{d,\sigma}(t) n_{d\sigma} + U\left(n_\uparrow - \frac{1}{2}\right)\left(n_\downarrow - \frac{1}{2}\right),$$



PHYSICAL REVIEW B **98**, 045404 (2018)

Anomalous Joule law in the adiabatic dynamics of a quantum dot in contact with normal-metal and superconducting reservoirs

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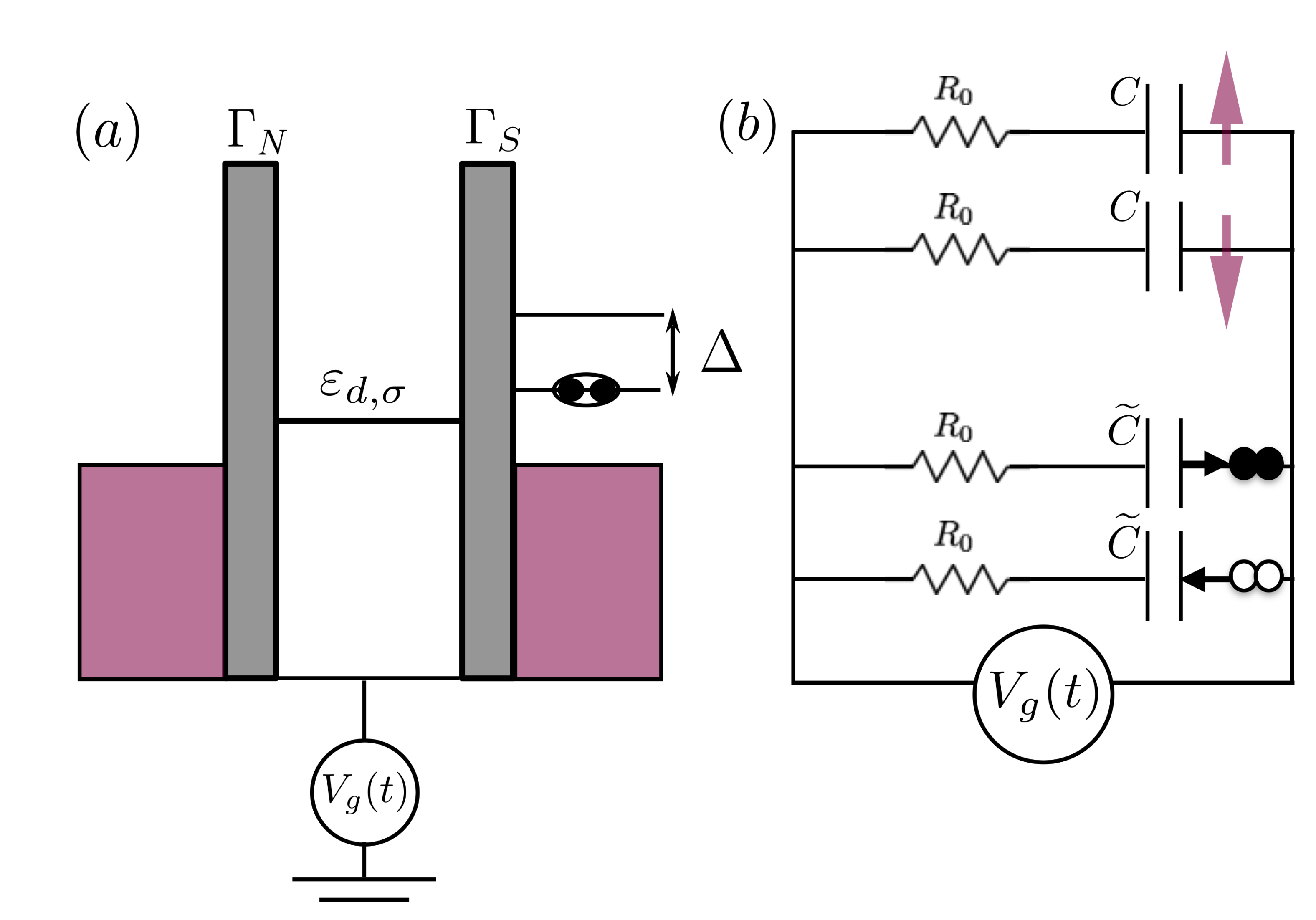


Also in this system the ER is necessary to get the Joule law

COLLABORATORS

- María Florencia Ludovico (ex PhD student), Francesca Battista (ex Postdoc), Javier Romero (ex Postdoc)
- Armando Aligia (Bariloche)
- Pablo Roura-Bas (Bariloche)
- Michael Moskalets (Karkhiv)
- David Sanchez and Rosa Lopez (Illes Balears)
- Felix von Oppen (Berlin)

CONICET

Ministerio de Ciencia, Tecnología e Innovación Productiva
Presidencia de la Nación

Alexander von Humboldt
Stiftung/Foundation

THANK YOU!

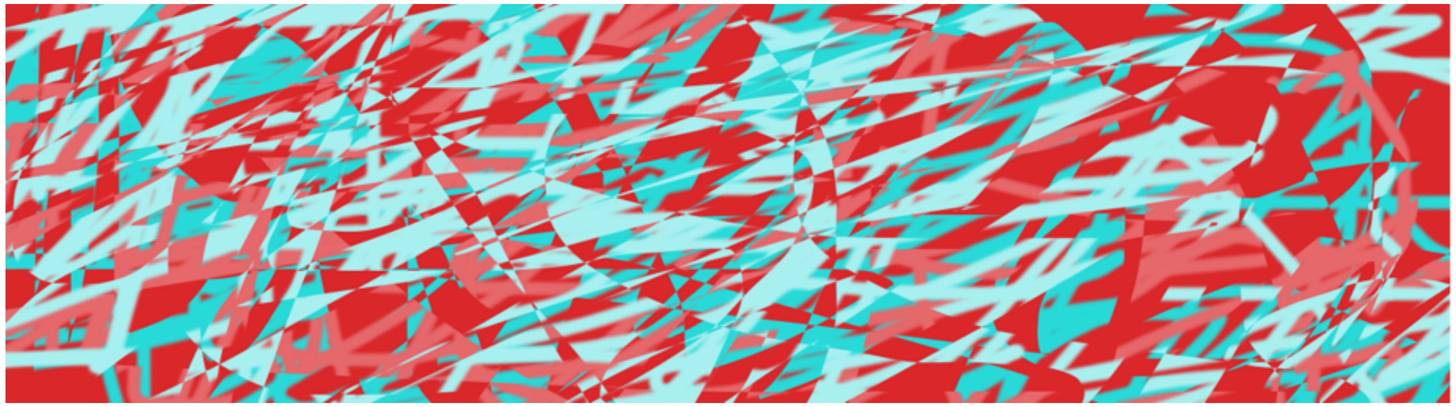
Xul Solar, Argentina, 1937-1963

QTTS (/)

Quantum Transport and Thermodynamics Society (/)

(/)

https://qtts.ifisc.uib-csic.es



A network of scientists dedicated to understanding the thermodynamics of quantum systems and quantum transport.

The theory of thermodynamics was the great success of 19th century physics. It has given enormous insight into how a machine turns heat into power, whether the machine is a steam engine or a nuclear power station. Similarly, it tells us how power can be used for refrigeration, from your household refrigerator to cooling circuits for superconducting MRI scanners in hospitals. It is a theory which tells us that disorder called *entropy* is at the heart of most physical processes, and that this disorder increases with time. This necessity that entropy increases with time is what ensures that heat cannot spontaneously flow from cold to hot, and why chemical reactions in your body go in one direction rather than another.

However, the theory of thermodynamics was developed more than 100 years ago, before we knew much about the quantum nature of small objects (electrons, atoms, molecules, etc); in particular that they can exhibit wave-particle duality, that they can be in two different states at the same time (superposition) and can be entangled with other quantum particles far away. All of these effects are described by the theory of quantum mechanics whose consequences are so far reaching that scientists have been grappling with them since the theory was invented in 1925. *Quantum transport* is the theory of how such quantum objects flow from one place to another, and how this flow is affected by wave-particle duality, superposition and entanglement. Most commonly the quantum objects that flow are electrons in metals, semiconductors or superconductors, but they could also be atoms in optical lattices.

The traditional theory of thermodynamics does not account for many of the above counter-intuitive quantum effects, so our aim is to develop theories which do. This is crucial, because we are now designing and building proto-type thermodynamic machines to turn heat into work (or vice versa), which can exhibit these quantum effects. Typically such machines consist of a few quantum objects, or involve flows of a few particles at a time, which makes the effects of wave-particle duality, superposition and entanglement very strong.

Our main objective is to better understand the laws of nature. More particularly, we aim to better understand what heat and entropy mean for quantum objects, and to better understand how such objects thermalize. We also aim to understand what quantum machines can be capable of, and what the laws of physics do not allow. At the same time, more practical goals include;

- Understanding how to measure heat flows and temperatures at the quantum scale.
- Using non-equilibrium thermodynamic measurements to tell us more about a quantum system that we are studying. For example, using the thermoelectric response of a quantum system to learn more about it.
- Using ideas from quantum transport and quantum thermodynamics to devise more efficient thermoelectrics and photovoltaics.