Quantum thermodynamics and transport Focus on heat-work conversion Lecture 3

Liliana Arrachea (2023)

Thermodynamic cycles





V





Heat-work conversion

$$W^{(\text{cons})} = Q_{\text{h}}^{(\text{qs})} \frac{(T_{\text{h}} - T_{\text{c}})}{T_{\text{h}}}$$

Power Finite-time efficiency W W $\eta = - \eta_C$ au_C



Single ion heat engine with maximum efficiency at maximum power

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$$\langle Q_2 \rangle = \langle H \rangle_C - \langle H \rangle_B = \frac{\hbar \omega_2}{2} \left[\coth\left(\frac{\beta_2 \hbar \omega_2}{2}\right) - Q_1^* \coth\left(\frac{\beta_1 \hbar \omega}{2}\right) \right]$$

$$\langle W_3 \rangle = \langle H \rangle_D - \langle H \rangle_C = \left(\frac{\hbar\omega_1}{2} Q_2^* - \frac{\hbar\omega_2}{2}\right) \coth\left(\frac{\beta_2 \hbar\omega_2}{2}\right)$$

Odd isochore: $D(\omega_1, \beta_2) \rightarrow A(\omega_1, \beta_2)$

$$\langle Q_4 \rangle = \langle H \rangle_A - \langle H \rangle_D = \frac{\hbar \omega_1}{2} \left[\coth\left(\frac{\beta_1 \hbar \omega_1}{2}\right) - Q_2^* \coth\left(\frac{\beta_2 \mu_2}{2}\right) \right]$$

A single-atom heat engine

Johannes Roßnagel,^{1,*} Samuel Thomas Dawkins,¹ Karl Nicolas Tolazzi,¹ Obinna Abah,² Eric Lutz,² Ferdinand Schmidt-Kaler,¹ and Kilian Singer^{1,3}

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Science 352, 325 (2016)



Simplifications of the "Otto description"

- heat is exchanged.
- the contacts to the baths.

• Perfect separation of strokes where only work or only

• The time-dependent processes of switching on and off

Pumping

Archimides screw





Archimedes Pump







Two operations

Generator





EUROPHYSICS LETTERS

14 January 1992 published in December 1991

Europhys. Lett., 17 (3), pp. 249-254 (1992)

Single-Electron Pump Based on Charging Effects.

H. POTHIER, P. LAFARGE, C. URBINA, D. ESTEVE and M. H. DEVORET

Service de Physique de l'Etat Condensé, Centre d'Etudes de Saclay 91191 Gif-sur-Yvette, France



Charge pumping

Fig. 1. – Principle of reversible transfer of a single electron using a «pump» controlled by two gate voltages U_1 and U_2 . a) Circuit schematic: the nanoscale junctions constituting the pump are represented by double-box symbols. b) Stable configuration diagram for V = 0 and C = C' = C''. One turn around a triple point such as P or N, obtained by modulating the gate voltages by two phaseshifted signals, induces one electron to go around the circuit.



PHYSICAL REVIEW B

VOLUME 58, NUMBER 16

Scattering approach to parametric pumping

P. W. Brouwer Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138

Pumped current

D. J. Thouless, Quantization of particle transport, Phys. Rev. B 27, 6083 (1983).

15 OCTOBER 1998-II



At least two parameters are needed!

J. E. Avron, A. Elgart, G. M. Graf, and L. Sadun, Optimal Quantum Pumps, Phys. Rev. Lett. 87, 236601 (2001).



www.sciencemag.org SCIENCE VOL 283 19 MARCH 1999

An Adiabatic Quantum **Electron Pump**

M. Switkes,¹ C. M. Marcus,¹* K. Campman,² A. C. Gossard²









PHYSICAL REV

Floquet scattering

M. Moskale

where B 66, 205320 (2002)
g theory of quantum pumps

$$A \xrightarrow{E}_{B} \xrightarrow{F}_{G} \xrightarrow{F}_{G}$$

$$A \xrightarrow{E_{n} = E + n\hbar\Omega}_{-a} \xrightarrow{-a}_{+a} \xrightarrow{+a}_{Adiabatic description (small E_{n})} \qquad S_{\alpha\beta,t}(E) + S_{\alpha\beta}^{(ad)}(E), \qquad S_{\alpha\beta}^{(ad)}(E) \propto C_{\alpha\beta}^{(ad)}(E) \propto C_{\alpha\beta}^{(ad)}($$

Floquet scatterin $S_{F,\alpha\beta}(E,I)$

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 Moskalets³









Cours/Lecture Series

https://cds.cern.ch/record/282618/files/AT00000125.pdf

1992 – 1993 ACADEMIC TRAINING PROGRAMME

LECTURE SERIES

: Michael BERRY / University of Bristol **SPEAKER** : Geometric Phases TITLE TIME

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: Auditorium PLACE



ABSTRACT

An elementary account will be given of the mathematical phenomenon of "global change without local change", i.e. anholonomy, applied to phases in quantum mechanics and angles in classical mechanics. Phases and angles in photons, electrons, and molecules will be discussed, with a historical emphasis. More advanced topics may include a detailed illustration of the vector and scalar gauge forces associated with the geometric reaction of a light system or a heavy one (modern Born-Oppenheimer theory) and high-order adiabatic corrections to the geometric phase and its relation to recent developments in asymptotics.

geometric phase : independent of T, dependent only my n and the geometry of C; system's answer to: "where have you been?" Yn(C) is phase anholonomy As with other currinit dependent quantities in physics, 8n(C) = flux of something through C (e.g. emf = flux of rate of change of magnetic field) Mere (from Schrödinger equation) $\mathcal{Y}_n(c) = - \int \int Im \langle dn \rangle_n | dn \rangle$ abstractly $\frac{\partial \psi^{*}(z;X)}{\partial X_{i}} \frac{\partial \psi^{*}(z;X)}{\partial X_{i}} - \frac{\partial \psi^{*}(z;X)}{\partial X_{i}} \frac{\partial \psi^{*}(x;X)}{\partial X_{i}} + \frac{\partial \psi^{*}(x;X)}{\partial X_{i}$ dX,dX_ [[[dr Im] J=S=C coordinates spanning C Concrete



Motors



Finite-time thermodynamic cycles in continuous coupling to the baths

Editors' Suggestion

Featured in Physics

Geometric properties of adiabatic quantum thermal machines

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Operational modes



Operational Regime

- Adiabatic: Time scale of the driving much larger than any other internal time scale of the small quantum system, including the relaxation time with the reservoirs (Small \hat{X})
- Small temperature difference between the two reservoirs. (Small $\Delta T/T$)

with linear response in $\Delta T/T$

Ideal scenario to combine adiabatic linear response in X

 $\mathcal{H}_{baths} = \mathcal{H}_{R} + \mathcal{H}_{L}$ $\mathcal{H}_{S}(t) \equiv \mathcal{H}_{S}[\vec{X}(t)]$ $\dot{X}(t) = \{X_{\ell}(t)\}$ $\ell = 1, \ldots, N$

Hamiltonian

Contacts between system and baths

$\mathcal{H}(t) = \mathcal{H}_{S}(t) + \mathcal{H}_{baths} + \mathcal{H}_{c} + \mathcal{H}_{th}(t).$

Luttinger Hamiltonian to represent thermal bias

Luttinger approach

J. M. Luttinger, Theory of thermal transport coefficients, Phys. Rev. 135, A1505 (1964). Phys. Rev. Lett. 114,196601 (2015).

$$\mathcal{H}_{\rm th}(t) = -\sum_{\alpha=L,R} \mathcal{J}^E_{\alpha}(t) \xi_{\alpha}$$

Lead
 $\dot{\xi}_{\alpha}(t) = \delta T_{\alpha}(t)/T$. and t
(Kub

G. Tatara, Thermal Vector Potential Theory of Transport Induced by a Temperature Gradient,

ls to proper results for heat thermoelectric current in linear response o) formalism upon carefully treating the *'diamagnetic''* term.

Energy Flux and force operators $\frac{\Omega}{2\pi}$: period of the cycle

$\mathcal{J}^{E}_{\alpha} = \dot{\mathcal{H}}_{\alpha} = -i[\mathcal{H}_{\alpha}, \mathcal{H}]/\hbar. \longrightarrow$

 $\mathcal{F}_{\ell} = -\frac{\partial \mathcal{H}}{\partial X_{\ell}}, \quad \text{with } \ell = 1,$

$$J^{Q}_{\alpha} = \frac{\Omega}{2\pi} \int_{0}^{2\pi/\Omega} dt \langle \mathcal{J}^{E}_{\alpha} \rangle$$

...,
$$N \longrightarrow \mathcal{F} = (\vec{\mathcal{F}}, \mathcal{J}_{R})^{T}$$

Energy flux operator
into the cold reservoir

Adiabatic linear response

Recall: Adiabatic susceptibilities are evaluated wrt the equilibrium frozen Hamiltonian

Adiabatic forces

 $F_{\ell}(t) = F_{\ell,t} + \sum_{\ell,\ell'} \Lambda_{\ell,\ell'}(\vec{X}) \dot{X}_{\ell'} + \Lambda_{\ell,N+1}(\vec{X}) \frac{\Delta T}{T}$ *ℓ*′=1 $J^{Q}(t) = \sum_{N+1,\ell'}^{N} (\vec{X}) \dot{X}_{\ell'} + \Lambda_{N+1,N+1}(\vec{X}) \frac{\Delta T}{T}$ $\ell'=1$

Thermal geometric tensor: $\Lambda_{\mu,\nu}(X)$ $\mu,\nu=1,\ldots,N+1$

Onsager relations

In many examples

 $\Lambda_{\ell,\ell'}(\overrightarrow{X}) = \Lambda_{\ell',\ell}(\overrightarrow{X}), \qquad \ell,\ell' = 1,...,N$

 $\Lambda_{\mu\nu}(\vec{X}, B) = \pm \Lambda_{\nu\mu}(\vec{X}, -B)$

Notation

 $\overrightarrow{\Lambda}(\overrightarrow{X}) = \left(\Lambda_{N+1,1}(\overrightarrow{X}), \dots, \Lambda_{N+1,N}(\overrightarrow{X})\right)$

 $\kappa = \Lambda_{N+1,N+1}(X)$

Heat engine Heat-work conversion

$W_{\rm out/in} = -Q_{\rm pump} \frac{\Delta T}{T}$

Highlight (I)

Heat-work conversion term is the counterpart of work produced in usual Carnot cycle (limit of zero dissipation)

Highlight (II) $W_{\text{out/in}} = -Q_{\text{pump}} \frac{\Delta T}{T}$ $\overrightarrow{\Lambda}(\overrightarrow{X}) = \left(\Lambda_{N+1,1}(\overrightarrow{X}), \dots, \Lambda_{N+1,N}(\overrightarrow{X})\right) \quad \text{~Berry connection}$

At least two control parameters are necessary to have a non-vanishing value!

$\mathcal{H}_{S}(t) = \vec{B}(t) \cdot \hat{\vec{\sigma}}.$ $\vec{B}(t) = (B_x(t), 0, B_z(t)),$

 $\mathcal{H}_{\alpha} = \sum \varepsilon_{k\alpha} b_{k\alpha}^{\dagger} b_{k\alpha}, \quad \alpha = L, R,$

 $\mathcal{H}_{c,\alpha} = \sum V_{k\alpha} \hat{\tau}_{\alpha} (b_{k\alpha} + b_{k\alpha}^{\dagger}),$

 $\hat{\tau}_L = \hat{\sigma}_x$ and $\hat{\tau}_R = \hat{\sigma}_z$.

Energy current:

 $J_{\alpha}^{f/a}(t) = \operatorname{Tr} \left[H_{\mathrm{S}}(\vec{X}) \mathcal{L}_{\alpha} \left[\hat{\rho}^{(f/a)} \right] \right]$

Solution with master equations: weak coupling

Adiabatic correction

$$, \hat{\rho}^{(f)}] + \sum_{\alpha} \mathcal{L}_{\alpha} \left[\hat{\rho}^{(f)} \right]$$

$$= \sum_{\alpha} \mathcal{L}_{\alpha} \left[\hat{\rho}^{(\alpha)} \right]$$

Geometric optimization of non-equilibrium adiabatic thermal machines and implementation in a qubit system

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Phys. Rev. X Quantum 3, 010326 (2022)

Heat engine

Pumping

$$\vec{X}(t) \equiv \vec{B}(t)$$
$$t = \tau \theta$$
$$\vec{B}(t) = \vec{B}(\theta \tau), \quad \theta \in [0, 1]$$

"Berry" Curvature

$$A = \int_{\partial \Sigma} \vec{\Lambda} \cdot d\vec{B} = \int_{\Sigma} (\vec{\nabla}_B \wedge \vec{\Lambda}) \cdot d\vec{B}$$

Thermodynamic length

$$L^{2} \geq \left(\int_{0}^{1} d\theta \sqrt{\vec{B} \cdot \underline{\Lambda} \cdot \vec{B}} \right)^{2} \equiv \mathcal{L}^{2}$$

Heat conductance $\langle \kappa \rangle = \int_0^1 d\theta \kappa$

Power and efficiency of the heat engine $\frac{W}{\tau} = \frac{\Delta T}{T} \frac{A(1 - \frac{\tau_D}{\tau})}{\tau}$ $\eta = \frac{W}{Q} = \eta_C \frac{1 - \frac{\tau_D}{\tau}}{1 + \frac{\tau}{\tau_L}}, \qquad \tau_D = \frac{T}{\Delta T} \frac{L^2}{A}, \quad \tau_\kappa = \frac{T}{\Delta T} \frac{A}{\langle \kappa \rangle}$

Maximal Power and efficiency

Optimizing with respect to the duration of the cycle:

$$P_{\max} = \frac{1}{4} \frac{(\Delta T)^2}{T^2} \frac{A^2}{L^2} , \quad \eta_{P_{\max}} = \frac{\eta_C}{2} \frac{x-1}{x+1} \qquad x = 1 + \frac{A^2}{L^2 \langle \kappa \rangle}$$

Optimizing the power reduces to an isoperimetric problem: The task of finding the shape that maximizes the ratio between area and perimeter in a space with non-trivial metric.

Isoperimetric problem = **Cheeger problem**

Interesting open problem in geometry!

- Antonio Ros, "The isoperimetric problem," Global theory of minimal surfaces **2**, 175–209 (2001).
- Enea Parini, "An introduction to the cheeger problem," Surv. Math. Appl. 6, 9–21 (2011).
- Gian Paolo Leonardi, "An overview on the cheeger problem," New trends in shape optimization , 117–139 (2015).
- Viktor Blåsjö, "The Isoperimetric Problem," The American Mathematical Monthly **112**, 526–566 (2005).
- Hugh Howards, Michael Hutchings, and Frank Morgan, "The Isoperimetric Problem on Surfaces," The American Mathematical Monthly **106**, 430–439 (1999).
- Frank Morgan, "Manifolds with density," Notices of the AMS **52**, 853–858 (2005).
- César Rosales, Antonio Cañete, Vincent Bayle, and Frank Morgan, "On the isoperimetric problem in Euclidean space with density," Calculus of Variations and Partial Differential Equations **31**, 27–46 (2007).
- Colin Carroll, Adam Jacob, Conor Quinn, and Robin Walters, "THE ISOPERIMETRIC PROBLEM ON PLANES WITH DENSITY," Bulletin of the Australian Mathematical Society **78**, 177–197 (2008).

Results

This protocol saturates the bound $A = k_B T \log(2)$

Results:

 $\max A^2/\mathcal{L}^2$

Open problems

Connection with topology

Quantum geometry and bounds on dissipation in slowly driven quantum systems

Iliya Esin,¹ Étienne Lantagne-Hurtubise,¹ Frederik Nathan,^{1,2} and Gil Refael¹

$$H(t) = h_0(t) + \mathbf{d}(t) \cdot \boldsymbol{\sigma}$$

Two-frequency driving: $\phi_1(t) = \omega_1 t$, $\phi_2(t) = \omega_2 t$

Net work conversion:

$$\overline{W}_{c} = \frac{\omega_{1}\omega_{2}}{T} \int_{0}^{T} dt \left[\frac{\tau_{2}^{2}\Delta^{2}}{1 + \tau_{2}^{2}\Delta^{2}} \right] \Omega_{1}$$

arXiv: 2306.17220

12,

Berry curvature: $\Omega_{12} = \frac{1}{2} \mathbf{d} \cdot \left(\partial_{\phi_1} \hat{\mathbf{d}} \times \partial_{\phi_2} \hat{\mathbf{d}} \right)$

Spin-boson problem out of equilibrium

ARTICLE

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OPEN

Probing the strongly driven spin-boson model in a superconducting quantum circuit

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Corrected: Publisher correction

Take-home message

- Quantum systems operating under periodic driving in contact to two thermal reservoirs at different temperatures may operate as thermal machines: engines or refrigerators if and only if there exist a heat-work conversion mechanism.
- For slow driving such mechanism is associated to pumping and it is described by a geometric quantity akin to a Berry phase.
- Useful for optimizing protocols in combination with the thermodynamic length.

Collaborators

- PhD Students:, Juan Herres Gerónimo Caselli
- Ex students/postdocs: Daniel Gresta, Pablo Terren Alonso, Leonel Gruñeiro, Gianmichele Blasi, Bibek Bhandari, Florencia Ludovico, Nastaran Dashi, Paolo Abiuso, Francesca Battista, Javier Romero
- Christian Reichl, Werner Wegscheider, Werner Diestche (ETH-Zürich), Jürgen Weiss (MPI-Stuttgart), Mariano Real (Buenos Aires), Alejandra Tonina, Paula Giudici (Buenos Aires)
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Reports on Progress in Physics

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Review

Energy dynamics, heat production and heat–work conversion with qubits: toward the development of quantum machines

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Thank you!

Xul Solar, Argentina, 1937-1963

Optimal driving for a given trajectory

FIG. 8. Power (blue) and efficiency (orange) for curve (b) of Fig. 6 as a function of the cycle duration τ . Solid lines: circulating around the curve at constant angular velocity. Dashed lines: Using the optimal velocities given by Eqs. (13) (for power) and (38) (for efficiency).

Adiabatic forces

 $\Lambda_{\mu,\nu}(\vec{X}) = \begin{cases} \chi_t^{\mathrm{ad}}[\mathcal{F}_{\mu},\mathcal{F}_{\nu}] & \mu \leq N & \dot{\vec{X}}(t) \\ \sum_{\alpha=L,R} \chi_t^{\mathrm{ad}}[\mathcal{J}_{\alpha}^E,\mathcal{F}_{\nu}] & \mu=N+1 & \dot{X}_{N+1}(t) = \Delta T(t)/T \end{cases}$ $\chi_{t}^{\mathrm{ad}} [\mathcal{F}_{l}, \mathcal{J}_{\alpha}^{E}] = -\chi_{t}^{\mathrm{ad}} [\mathcal{F}_{l}, \mathcal{J}_{\bar{\alpha}}^{E}],$ $\chi_{t}^{\mathrm{ad}} [\mathcal{J}_{\alpha}^{E}, \mathcal{F}_{l}] = -\chi_{t}^{\mathrm{ad}} [\mathcal{J}_{\bar{\alpha}}^{E}, \mathcal{F}_{l}],$

 $\langle \mathcal{F} \rangle(t) = \langle \mathcal{F} \rangle_t + \underline{\Lambda}(\vec{X}) \cdot \mathbf{X}.$

