GEOMETRICAL QUANT
CHEMICAL ENGINE

Hisao Hayakawa ersity)
collaboration with anyo-Onoda
and Ville M. M. Pa ku)

2021-12-03
Nonequilibrium Phenomena in Driven Dissipative Sysyems
@YITP, Kyoto Univ.

YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

Contents

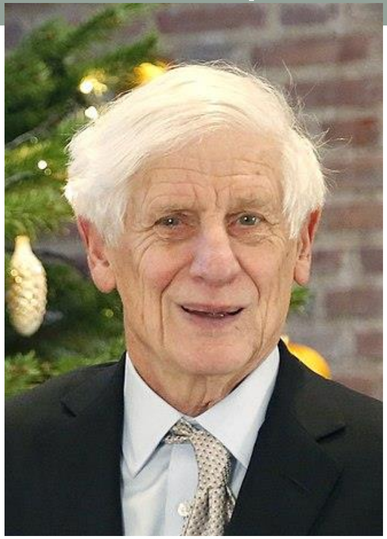
- Introduction
  - Thouless pumping and Berry's phase
  - Trade-off relation of thermodynamic engines
- Geometric Formulation to "thermodynamics" in quantum chemical engines
- Application to Anderson model
- Discussion and conclusion

Contents

- Introduction
  - Thouless pumping and Berry’s phase
  - Trade-off relation of thermodynamic engines
- Geometric Formulation to “thermodynamics” in quantum chemical engines
- Application to Anderson model
- Discussion and conclusion

Introduction

- I am talking on geometric pumping proposed by D. Thouless (1983) who got the Nobel prize in 2016.
- The essence of Thouless pumping is Berry’s phase proposed by M. Berry (1984).
- The idea by two big shots can be applied to non-equilibrium driven systems.
- Design of (thermodynamic) engines will be important.



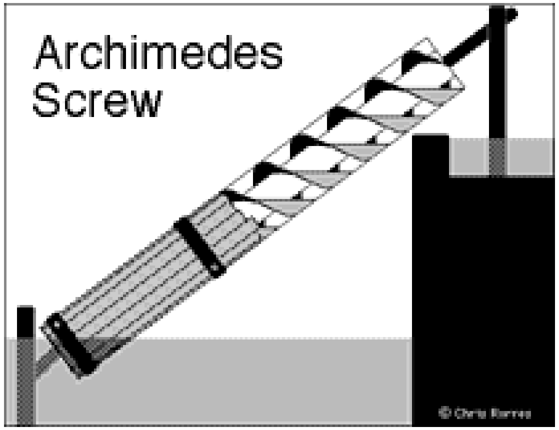
Photos taken from wikipedia

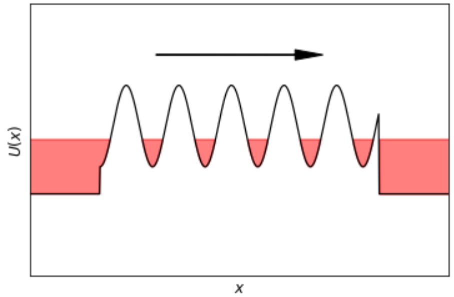
YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

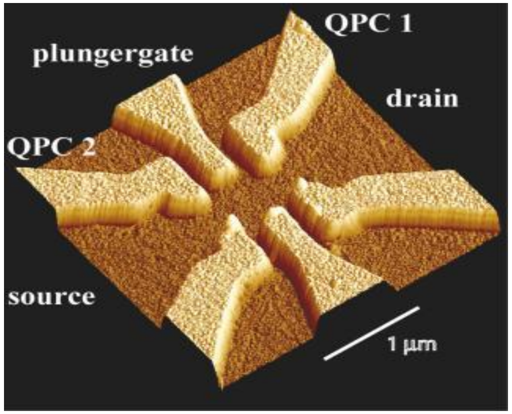
Pumping process

- Pump=>We need a bias.

The current can flow in a mesoscopic system without dc bias =>*Geometric (Thouless) pumping*.



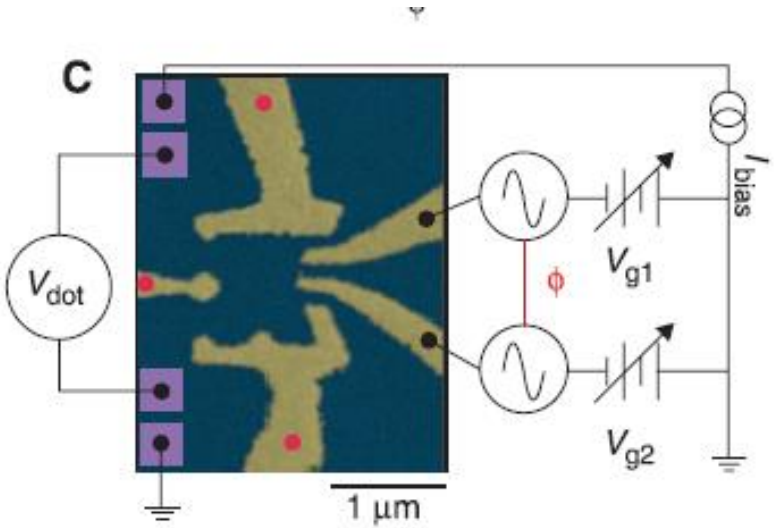


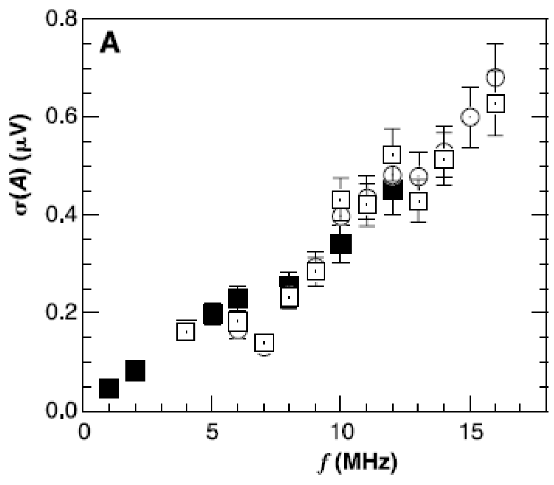


A nano-machine to extract a work

Previous studies

- Experiments
  - Pothier et al. (1992) get a classical pumping for a mesoscopic system.
  - Switkes et al. (1999) control the gate voltage and get 20 electrons current per a cycle in a quantum dot system.

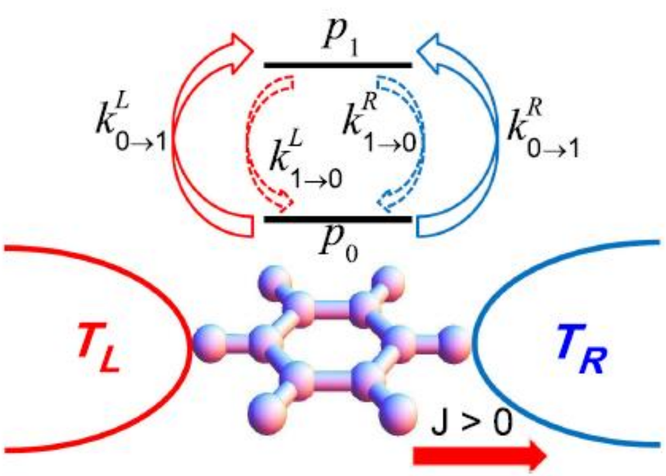


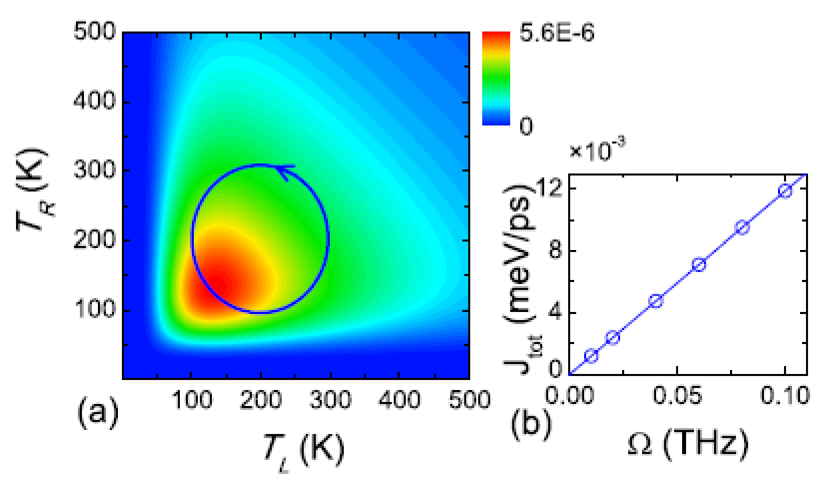


YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

Previous theoretical studies

- Adiabatic geometric pumping (theories)
  - Thouless (1983) for a closed system
  - Open quantum system (P. W. Brower (1998)).
- Sintsyin & Nemenman (2007) indicated that Berry's phase can be used to nonequilibrium stochastic processes.
- Ren-Hänggi-Li (2010) analyzed a spin-boson system and to clarify the role of Berry's phase.





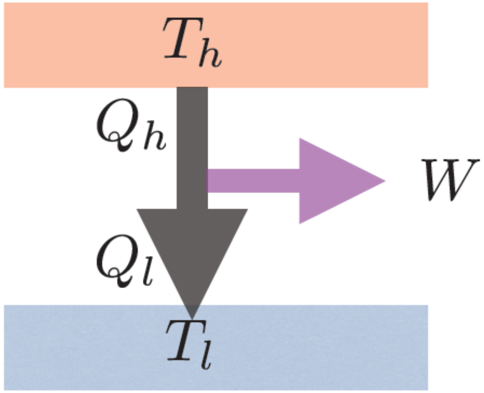
Trade-off relation between power & efficiency

- Power and efficiency

  - What is the limitation on the power and efficiency ?

Efficiency (textbook)

$$\eta := \frac{W}{Q_h} \leq 1 - T_l/T_h$$



$$W = Q_h - Q_l$$

Power

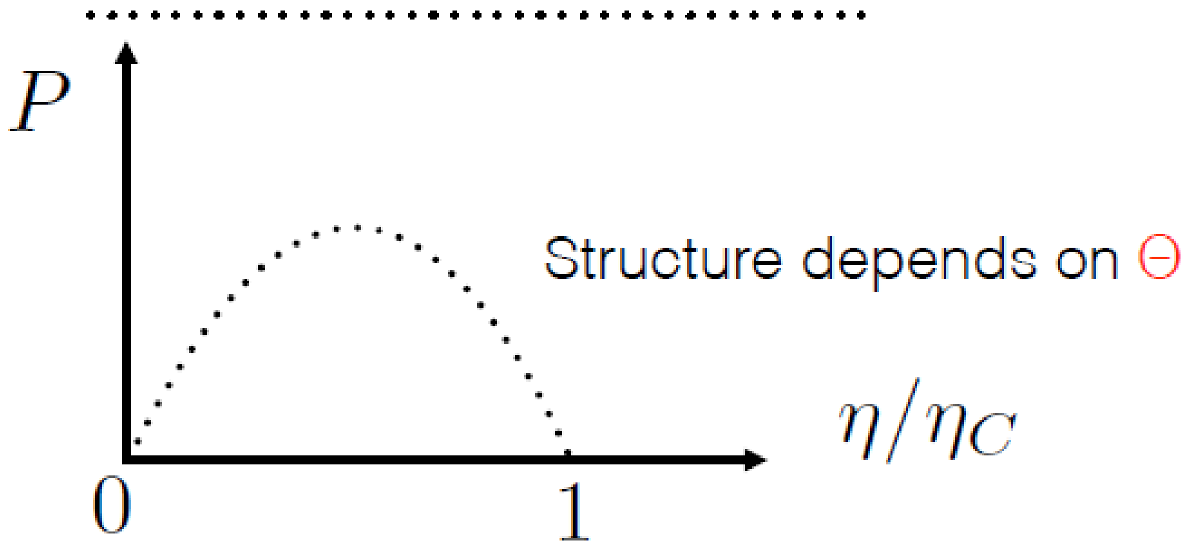
$P := W/\tau$ τ : period of the cycle

Generally, power is zero for the case of the highest efficiency.
=>It is practically useless.

Trade-off relation: part 2

- Shiraishi-Saito-Tasaki (2016) gave the trade-off relation for small amplitude and low speed case in Markovian dynamics.

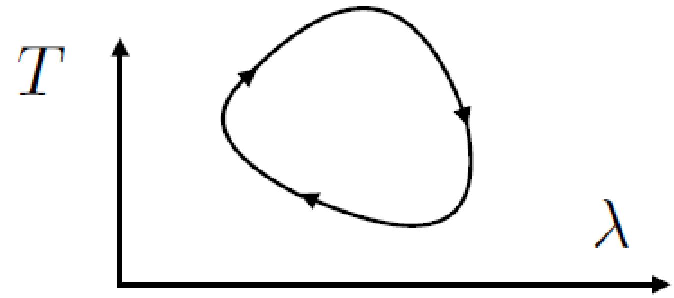
$$\Theta \beta_l (\eta/\eta_C)[1-(\eta/\eta_C)] \geq P$$



Trade-off relation part 3

YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

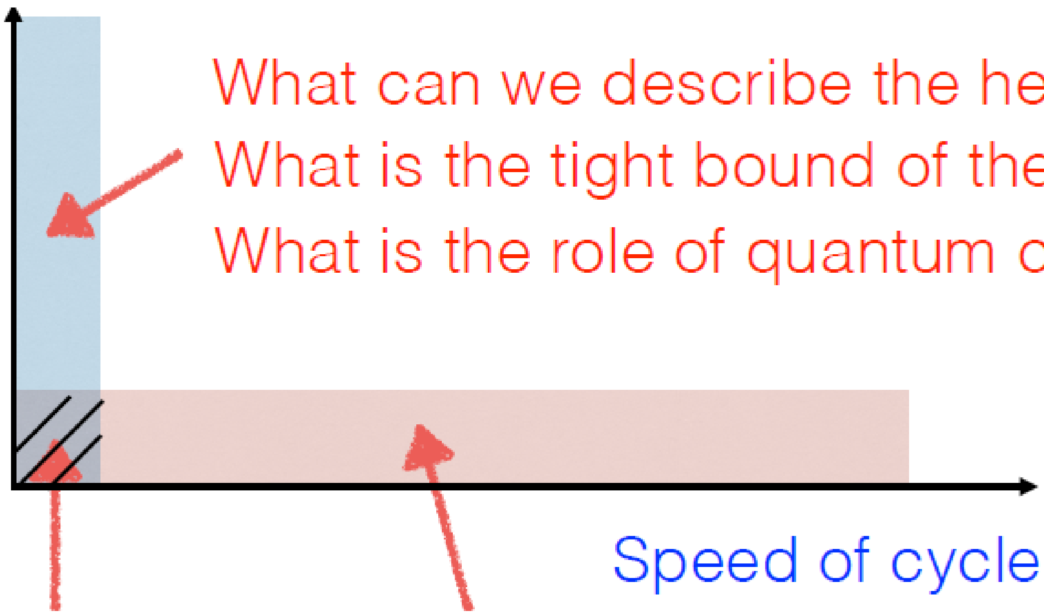
Amplitude of (λ, T)



What can we describe the heat engines ?

What is the tight bound of the power vs. efficiency ?

What is the role of quantum coherence ?



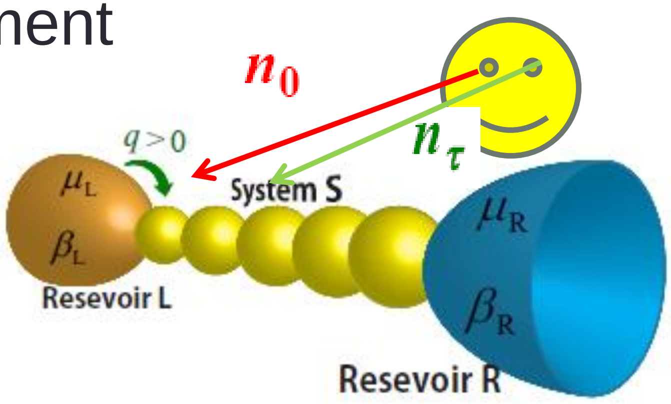
Large amplitude engines

- Brander & Saito, PRL **124**, 040602 (2020) implemented a heat engine with large amplitude.
  - They clarified the role of geometrical metric tensor.
  - They still assumed that there is only one reservoir.
- Heat engines controlled by multiple reservoirs associated with Thouless pumping was implemented by Hino & Hayakawa, PRR **3**, 013187 (2021).
- Let us discuss a quantum chemical engine by controlling the chemical potentials.
  - Extension of the previous works
  - Establishment of quantum engines which are easy to be implemented.

Contents

Setup

- Projection measurement



- Control parameters
  - Chemical potentials in heat reservoirs
  - One parameter in the system Hamiltonian to extract the work

Chemical Engines

- We control chemical potentials μ_L and μ_R as well as the system Hamiltonian $\widehat{H}(\lambda(\theta))$ through a control parameter$\lambda(\theta)$ depending on the phase of modulationθ.
- Quantum master equation for the density matrix $\hat{\rho}$

$$\frac{d}{d\theta}|\hat{\rho}(\theta)\rangle = \epsilon^{-1}\hat{K}(\mathbf{\Lambda}(\theta))|\hat{\rho}(\theta)\rangle,$$

$$\mathbf{\Lambda} := \left(\lambda, \frac{\mu^{\mathrm{L}}}{\overline{\mu^{\mathrm{L}}}}, \frac{\mu^{\mathrm{R}}}{\overline{\mu^{\mathrm{R}}}}\right) \qquad \overline{\mu^{\alpha}} := \frac{1}{\tau_p}\int_0^{\tau_p} dt \mu^{\alpha}(t)$$

$$\epsilon := 1/(\tau_{\mathrm{p}}\Gamma) \qquad \theta := 2\pi(t - t_0)/\tau_{\mathrm{p}}$$

Γ is the coupling strength

KL divergence

- Kullback-Leibler (KL) divergence

$$S^{\mathrm{KL}}(\hat{\rho}||\hat{\rho}^{\mathrm{ss}}) := \mathrm{Tr}[\hat{\rho}(\ln\hat{\rho} - \ln\hat{\rho}^{\mathrm{ss}})],$$

satisfies $S^{\mathrm{KL}}(\hat{\rho}||\hat{\rho}^{\mathrm{ss}}) \geq 0.$

- Then entropy production $\sigma := \frac{1}{2\pi}\int_0^{2\pi} S^{\mathrm{KL}}(\theta)d\theta \geq 0$

- If the dynamics is CPTP, $\dot{S}^{KL} \leq 0$:

$$\begin{aligned}\Delta S :&= -S^{\mathrm{KL}}(\hat{\rho}(2\pi)||\hat{\rho}^{\mathrm{ss}}(2\pi)) + S^{\mathrm{KL}}(\hat{\rho}(0)||\hat{\rho}^{\mathrm{ss}}(0))\\ &= -\int_0^{2\pi} d\theta \dot{S}^{\mathrm{KL}}(\hat{\rho}(\theta)||\hat{\rho}^{\mathrm{ss}}(\theta)) \geq 0\end{aligned}$$

Work relations

- We can introduce the “work” (see Jarzynski 1997)

$$W := \frac{1}{2\pi}\int_0^{2\pi} \mathrm{Tr}\left[\hat{\rho}(\theta)\frac{\partial \hat{H}(\lambda(\theta))}{\partial \lambda(\theta)}\right]\dot{\lambda}(\theta)d\theta$$

- This satisfies $W = E - T\sigma \leq E,$

E: corresponding to incoming heat

- W can be negative.
- If we require $\dot{\lambda} \geq 0$ and $\mathrm{Tr}[\hat{\rho}(\theta)\partial \hat{H}(\lambda(\theta))/\partial\lambda] \geq 0$, $W \geq 0$.
- We can introduce the efficiency and power

$$\eta^{\mathrm{eff}} := \frac{W}{E} = \frac{W}{W + T\sigma}. \qquad P := \epsilon W$$

Linear response regime

- If we are interested in slow modulations, we can use

$$\hat{\rho}(\theta) = \hat{\rho}^{\mathrm{ss}}(\theta) + \epsilon\hat{\rho}^{(1)}(\theta) + O(\epsilon^2)$$

$$S^{\mathrm{KL}}(\hat{\rho}||\hat{\rho}^{\mathrm{ss}}) = \frac{1}{2}\epsilon^2 \mathrm{Tr}\left[\hat{\rho}^{(1)}(\hat{\rho}^{\mathrm{ss}})^{-1}\hat{\rho}^{(1)}\right] + O(\epsilon^3)$$

$$\sigma = \epsilon^2\sigma^{(2)}$$

$$\sigma^{(2)} = \frac{1}{4\pi}\int_0^{2\pi} d\theta \mathrm{Tr}[\hat{\rho}^{(1)}(\hat{\rho}^{\mathrm{ss}})^{-1}\hat{\rho}^{(1)}]$$

$$\hat{\rho}^{(1)} := \partial_\nu \hat{\rho}^{\mathrm{ss}} \dot{\Lambda}_\nu \qquad |\partial_\nu \hat{\rho}^{\mathrm{ss}}(\mathbf{\Lambda}(\theta)\rangle := \hat{K}^{+}(\mathbf{\Lambda}(\theta))\frac{\partial}{\partial\Lambda_\nu(\theta)}|\hat{\rho}^{\mathrm{ss}}(\mathbf{\Lambda}(\theta))\rangle$$

Geometric expression

- We can rewrite

$$\sigma^{(2)} = \frac{1}{2\pi}\int_0^{2\pi} d\theta g_{\mu\nu}(\mathbf{\Lambda}(\theta))\dot{\mathbf{\Lambda}}_\mu(\theta)\dot{\mathbf{\Lambda}}_\nu(\theta),$$

$$g_{\mu\nu}(\mathbf{\Lambda}) := \frac{1}{2}\mathrm{Tr}[\partial_\mu \hat{\rho}^{\mathrm{ss}}(\mathbf{\Lambda})(\hat{\rho}^{\mathrm{ss}}(\mathbf{\Lambda}))^{-1}\partial_\nu \hat{\rho}^{\mathrm{ss}}(\mathbf{\Lambda})].$$

Fisher information

$$g_{\mu\nu} = \frac{1}{2}\mathrm{Tr}[\hat{\rho}^{\mathrm{ss}}\partial_\mu \ln \hat{\rho}^{\mathrm{ss}}\partial_\nu \ln \hat{\rho}^{\mathrm{ss}}]$$
$$= -\frac{1}{2}\mathrm{Tr}[\hat{\rho}^{\mathrm{ss}}\partial_\mu\partial_\nu \ln \hat{\rho}^{\mathrm{ss}}],$$

Hessian matrix

- Cramér–Rao bound: $Var(\Lambda_\mu) \geq g_{\mu\nu}^{-1}$: What does it mean?

Thermodynamic length

- Thermodynamic length

$$\mathcal{L} := \oint_{\partial\Omega} \sqrt{g_{\mu\nu}(\boldsymbol{\Lambda}) d\Lambda_\mu d\Lambda_\nu}$$
$$:= \frac{1}{2\pi}\int_0^{2\pi} d\theta \sqrt{g_{\mu\nu}(\boldsymbol{\Lambda}) \dot{\Lambda}_\mu(\theta) \dot{\Lambda}_\nu(\theta)}$$

- Inequality

$$\sigma^{(2)} \geq \beta \mathcal{L}^2$$

Work and vector potential

- The work is expressed as

$$\mathcal{W} := \oint_{\partial\Omega} \mathcal{A}_\mu(\mathbf{\Lambda}) d\Lambda_\mu = \int_\Omega d\mathcal{A}.$$

$$\mathcal{A}_\mu(\mathbf{\Lambda}) := \mathrm{Tr}\left[\frac{\partial \hat{H}}{\partial \lambda} \hat{\rho}^{\mathrm{ss}}(\mathbf{\Lambda})\right]$$

- Thermodynamic curvature $F_{\mu\nu} := \frac{\partial}{\partial \Lambda_\mu} A_\nu - \frac{\partial}{\partial \Lambda_\nu} A_\mu.$

- Thermodynamic axial field and flux $\mathscr{B}_\mu := \epsilon_{\mu\nu\rho} F_{\nu\rho},$

$$\Phi_{\mathrm{TD}} = \oint_{\partial\Omega} \mathcal{A}_\mu d\Lambda_\mu = \mathcal{W}. \qquad \Phi_{\mathrm{TD}} := \int_\Omega \vec{\mathscr{B}} \cdot d\vec{S},$$

Contents

- Introduction
  - Thouless pumping and Berry’s phase
  - Trade-off relation of thermodynamic engines
- Geometric Formulation to “thermodynamics” in quantum chemical engines
- Application to Anderson model
- Discussion and conclusion

Anderson model

- We consider Anderson model

$$\hat{H} = \sum_{\sigma} \epsilon_0 \hat{d}_\sigma^\dagger \hat{d}_\sigma + U(\theta)\hat{n}_\uparrow \hat{n}_\downarrow.$$

$$\hat{H}^{\mathrm{r}} = \sum_{\alpha,k,\sigma} \epsilon_k \hat{a}^\dagger_{\alpha,k,\sigma} \hat{a}_{\alpha,k,\sigma}$$

$$\hat{H}^{\mathrm{int}} = \sum_{\alpha,k,\sigma} V_\alpha \hat{d}^\dagger_\sigma \hat{a}_{\alpha,k,\sigma} + \mathrm{h.c.},$$

$$U(\theta) = U_0 \lambda(\theta), \quad \lambda(\theta) = \theta + r_\lambda \cos\theta, \qquad |r_\lambda| \le 1$$

- The wide band approximation

  =>quasi-classical

$$\hat{\rho} = \begin{pmatrix} \rho_d & 0 & 0 & 0 \\ 0 & \rho_\uparrow & 0 & 0 \\ 0 & 0 & \rho_\downarrow & 0 \\ 0 & 0 & 0 & \rho_e \end{pmatrix}$$

Eigenvalues and eigenvectors

- We can solve the eigenvalue problem exactly as

$$\hat{K}(\mathbf{\Lambda}(\theta)) = \begin{pmatrix} -2f_-^{(1)} & f_+^{(1)} & f_+^{(1)} & 0 \\ f_-^{(1)} & -f_-^{(0)} - f_+^{(1)} & 0 & f_+^{(0)} \\ f_-^{(1)} & 0 & -f_-^{(0)} - f_+^{(1)} & f_+^{(0)} \\ 0 & f_-^{(0)} & f_-^{(0)} & -2f_+^{(0)} \end{pmatrix}$$

$$f_+^{(j)} := f_L^{(j)}(\mu^L, U) + f_R^{(j)}(\mu^L, U)$$

$$f_+^{(j)} + f_-^{(j)} = 2$$

$$f_\alpha^{(j)}(\mu^\alpha(\theta), U(\theta)) := \frac{1}{1 + e^{\beta(\epsilon_0 + jU(\theta) - \mu^\alpha(\theta))}}$$

Explicit calculation

$$r := r_\lambda = r_\mu = r_T = 0.5$$

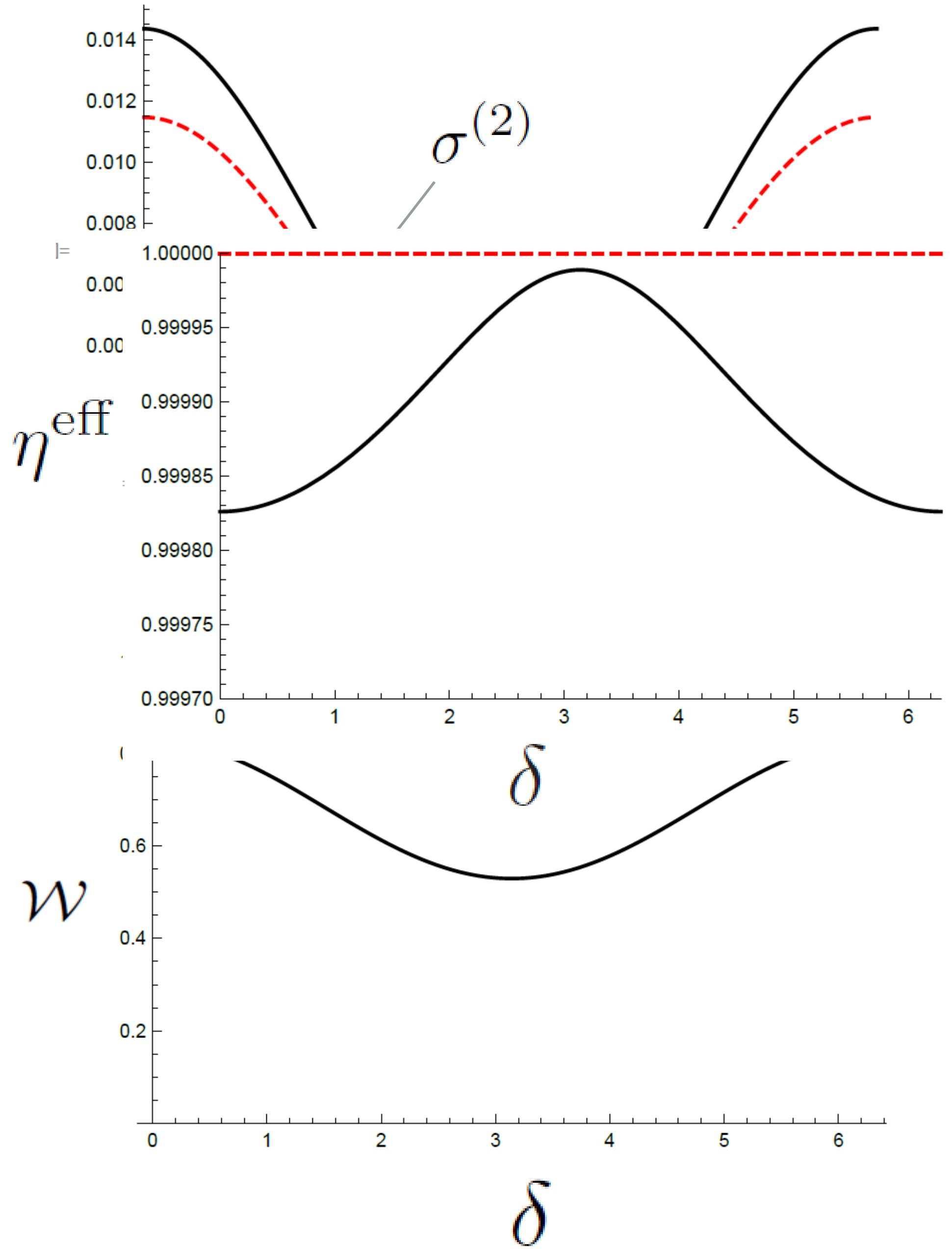
$$\lambda(\theta) = \theta + r_\lambda \cos\theta$$

$$\frac{\mu^{\mathrm{L}}(\theta)}{\overline{\mu}} = 1 + r_\mu \sin\theta,$$

$$\frac{\mu^{\mathrm{R}}(\theta)}{\overline{\mu}} = 1 + r_T \sin[\theta + \delta]$$

δ : the phase shift parameter of chemical potentials modulation

YUKAWA INSTITUTE FOR THEORETICAL PHYSICS



YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

Contents

- Introduction
  - Thouless pumping and Berry's phase
  - Trade-off relation of thermodynamic engines
- Geometric Formulation to "thermodynamics" in quantum chemical engines
- Application to Anderson model
- Discussion and conclusion

Discussion

- If we use $\Delta S := -S^{KL}(\rho(2\pi)||\rho^{ss}(2\pi)) + S^{KL}(\rho(0)||\rho^{ss}(0))$, it can be expressed as

$$\Delta S = \epsilon^2 \left[g_{\mu\nu}(0)\dot{\Lambda}_\mu(0)\dot{\Lambda}_\nu(0) - g_{\mu\nu}(2\pi)\dot{\Lambda}_\mu(2\pi)\dot{\Lambda}_\nu(2\pi) \right]$$

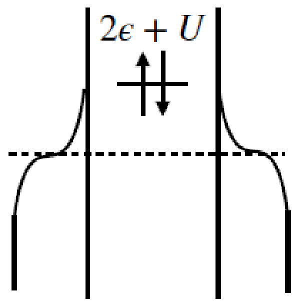
- If the system is completely periodic, ΔS=0.
  =>$\dot{S}^{KL}(\rho(\theta)||\rho^{ss}(\theta))$=0 for CPTP dynamics for all θ.
- => The system must not be completely periodic.
- If we control one of the temperatures in the reservoirs, we may consider the dissipative availability

$$A := -\int_0^{2\pi} d\theta \Theta(\theta) \dot{S}^{\mathrm{KL}}(\theta),$$

$\Theta(\theta)$ **is the modulated temperature** $\quad \bar{\Theta} = \bar{T}$

Discussion for perfectly cyclic modulation

Initial State



Modulation

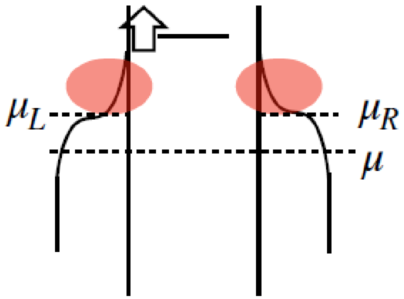
$$\mu_L = \mu(1 + \sin\theta)$$

$$\mu_R = \mu[1 + \sin(\theta + \delta)]$$

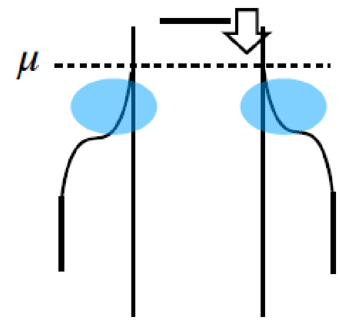
$$U = U_0[1 - \cos\theta]$$

Case of $\delta = 0$

$0 < \theta < \pi$



$\pi < \theta < 2\pi$



Larger # of electrons enters into QD

Larger # of electrons escape from QD

If energy inside QD increases ($\dot{\lambda} > 0$) for $0 < \theta < \pi$

and decreases ($\dot{\lambda} < 0$) for $\pi < \theta < 2\pi$

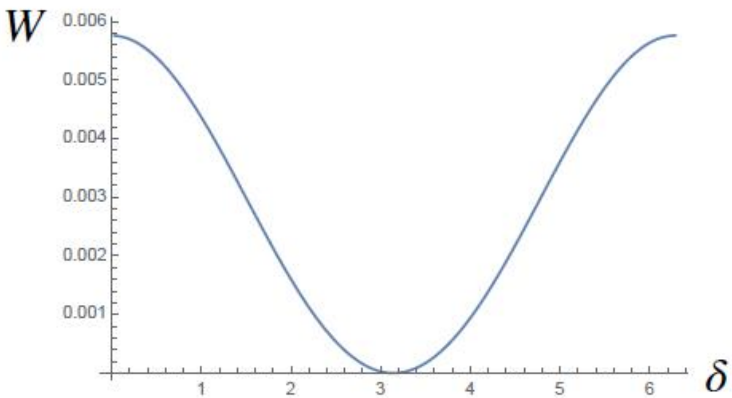
W becomes positive (it is correct for the present model)

Case of $\delta = \pi$

Even if energy inside QD increases ($\dot{\lambda} > 0$) for $0 < \theta < \pi$

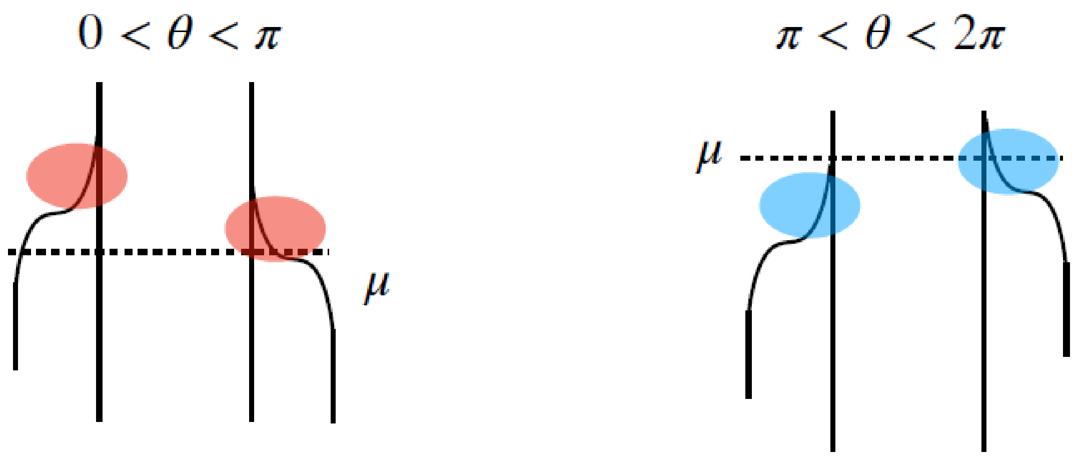
and decreases ($\dot{\lambda} < 0$) for $\pi < \theta < 2\pi$

W becomes 0 (gain and loss is compensated)

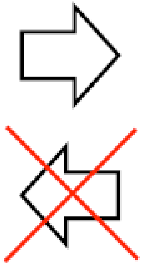


Speculation

General δ



If $\dot{\lambda} > 0$ for $\mu_L + \mu_R > 2\mu$ and $\dot{\lambda} < 0$ for $\mu_L + \mu_R < 2\mu$



W becomes non-negative

(Question: W can be interpreted as work?)

Future perspectives

YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

- The system we consider is not perfectly periodic. Why cannot we apply our formulation to such systems?
  - The efficiency can reach 1 without any difficulty for perfectly periodic systems. What does it mean?
- Entropy production rate might be more physical than the current formulation.=> What does it mean?
  - If we control the temperature of the reservoir, it is natural to use the dissipative availability.
- Our analyzed system is still quasi-classical. What happens in pure quantum systems?
- What happens if the operation speed is finite?

Summary

- We have formulated the description of geometrical pumping processes in terms of master equation.
- We have formulated a geometric thermodynamics to describe the quantum chemical and thermodynamic engines.
- We clarified that the geometric tensor (Fisher information or Hessian matrix) plays a key role.
- The vector potential is important for this system.
- It is still controversial how to use KL divergence.

YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

THANK YOU FOR YOUR ATTENTION.

Density matrix

- The density matrix is expressed as $\rho = \sum_{i=0}^{3} | r_i \ >< l_i |$.
- Since we have already known the left and right eigenvectors, we can calculate the density matrix easily.
- So we can calculate everything.

Perfectly periodic or quasi-periodic

- Perfectly periodic modulation does not lead positive semidefinite W.
  - If so, the engine does not satisfy the requirement of thermodynamics.
  - By definition, the entropy production must be zero after a cyclic modulation.
- Quasi-periodic modulation does not leads to periodic change of Hamiltonian.
  - This is strange in the sense of control.
  - This is natural in the thermodynamic sense.
  - We may miss some other quantity such as information.