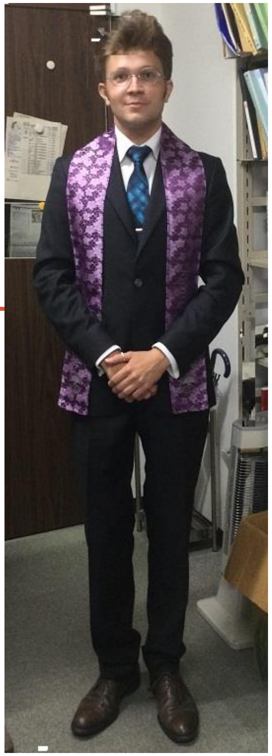
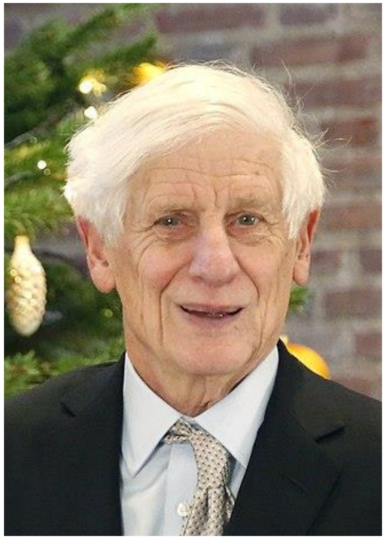
幾何学的量子化学エンジン

早川尚男　(京大基研)，
Ville M. M. Paasonen (Univ. Turku),
吉井涼輔（山口東京理科大）

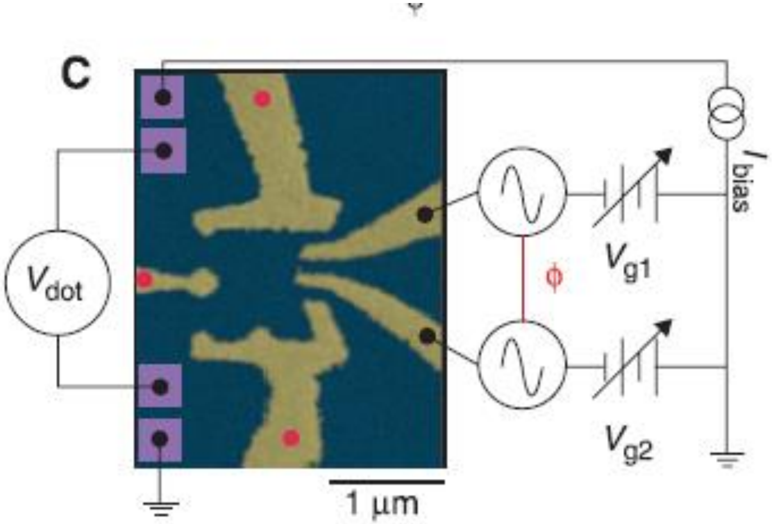


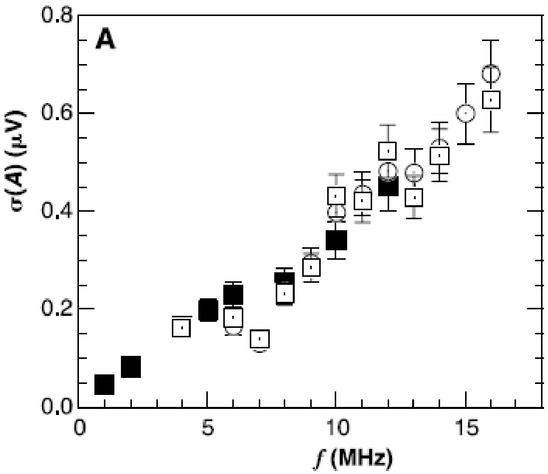
16aB14-3
日本物理学会@岡山大、2022年3月16日

Thouless pumping



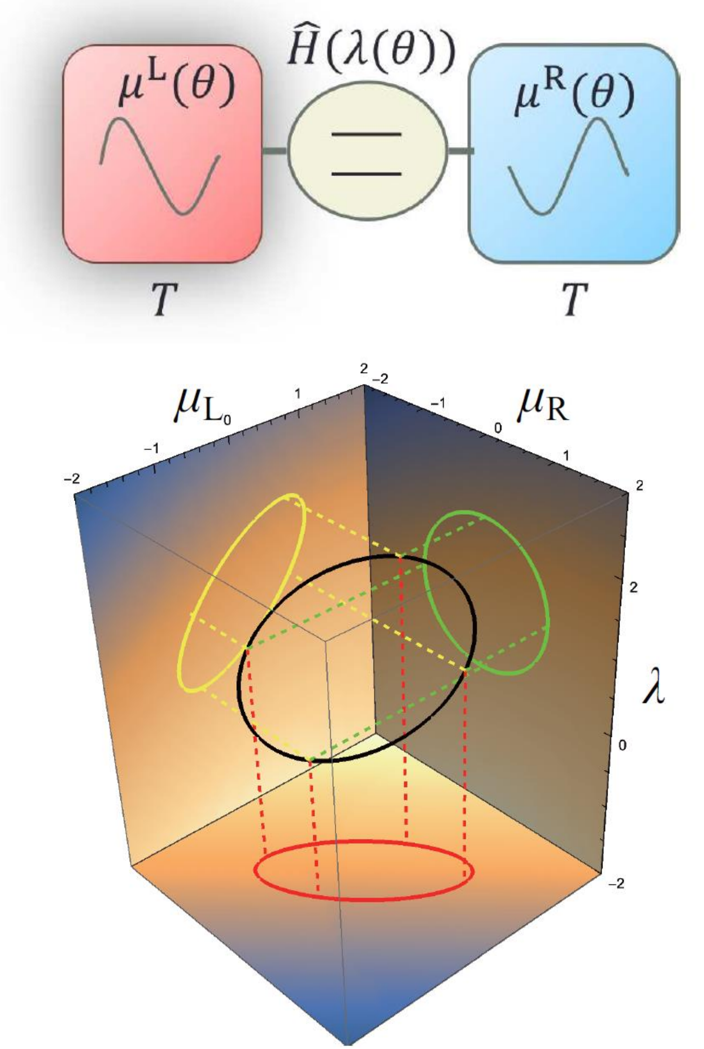
- Thouless (1983) proposed that current can flow without DC bias by the geometrical phase.
    - Pothier et al. (1992) and Switkes et al. (1999) control the gate voltage and get 20 electrons current per a cycle in a quantum dot system.





Geometrical engines

- Let us consider a small system sandwiched by two reservoirs.
- We control chemical potentials in the reservoirs and one parameter in the system Hamiltonian.
- The circular control of parameters=> geometric metric tensor
    - Brandner-Saito (PRL 2020) : one-reservoir
    - Hino-Hayakawa (PRR2021): two thermal reservoirs
- We want to implement the engine!



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 $\hat{\rho}$

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

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

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

Γ is the coupling strength

Relative entropy (Hatano-Sasa type)

- Hatano-Sasa type relative entropy

$$\boxed{S^{\rm HS}(\hat{\rho}||\hat{\sigma}) := {\rm Tr}\left[\hat{\rho}(\ln\hat{\rho} - \ln\hat{\sigma})\right]} \geq 0$$

- Non-cyclic modulation (Hayakawa et al. arXiv:2112.12370)
- Cyclic modulation (Yoshii & HH, in preparation)

$$\hat{H}(\lambda(\theta)) = \hat{H}(\lambda(\theta + 2\pi))$$

- If we begin with the NESS $|\hat{\rho}^{\rm SS}\rangle$, 1-cycle entropy change is

$$\Delta S := -S^{\rm HS}(\hat{\rho}(2\pi)||\hat{\rho}^{\rm SS}(2\pi)) + S^{\rm HS}(\hat{\rho}(0)||\hat{\rho}^{\rm SS}(0))$$

$$= -S^{\rm HS}(\rho(2\pi)||\hat{\rho}^{\rm SS}(2\pi)) \leq 0$$

- Thus, the entropy change is negative semidefinite, where the equality is only held $\rho = \rho^{SS}$.

Geometric expression of average of entropy

- We can rewrite the perturbation of entropy by ϵ

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

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

Fisher information

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

Hessian matrix

- The NESS is the maximum entropy state.

Geometrical state

$$|\hat{\rho}(0)\rangle = |r_0\rangle = |\hat{\rho}^{\mathrm{SS}}\rangle$$

$$\hat{K}|r_0\rangle = 0$$

- The density matrix satisfies

$$|\hat{\rho}(\theta)\rangle = |r_0(\theta)\rangle + \sum^{n} C_i(\theta)|r_i(\theta)\rangle,$$

$$C_i(\theta) = -\int_0^{\theta} d\phi e^{\epsilon^{-1}\int_\phi^\theta dz\epsilon_i(z)} \langle \ell_i(\phi)|\frac{d}{d\phi}|r_0(\phi)\rangle \sim O(\epsilon)$$

- The correction is the geometric term.
  - BSN connection

$$\mathcal{A}_i^{\mu} := -\langle \ell_i(\Lambda(\phi))|\frac{\partial}{\partial \Lambda_\mu}|r_0(\Lambda(\phi))\rangle, \quad \text{where } \Lambda_\mu \text{ is one of } (\mu_L, \mu_R, \lambda)$$

  - BSN curvature

$$F_i^{\mu\nu}(\theta) := \left(\frac{\partial \mathcal{A}_i^{\nu}}{\partial \Lambda_\mu}\right)_\theta - \left(\frac{\partial \mathcal{A}_i^{\mu}}{\partial \Lambda_\nu}\right)_\theta$$

Work relations

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

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

- Th heat

$$Q_{A/R} := \frac{1}{2\pi}\int_0^{2\pi} d\theta\, \mathscr{P}_{A/R}(\theta). \qquad \mathscr{P}_{A/R}(\theta) := \frac{\mathscr{P}(\theta) \pm |\mathscr{P}(\theta)|}{2}$$

- If W<0, the system becomes the engine.
- We can introduce the efficiency

$$\eta := \frac{|W|}{Q_A}$$

Anderson model

- For explicit calculation, we adopt the Anderson model

$$\hat{H}^{\mathrm{tot}} := \hat{H} + \hat{H}^{\mathrm{r}} + \hat{H}^{\mathrm{int}},$$

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

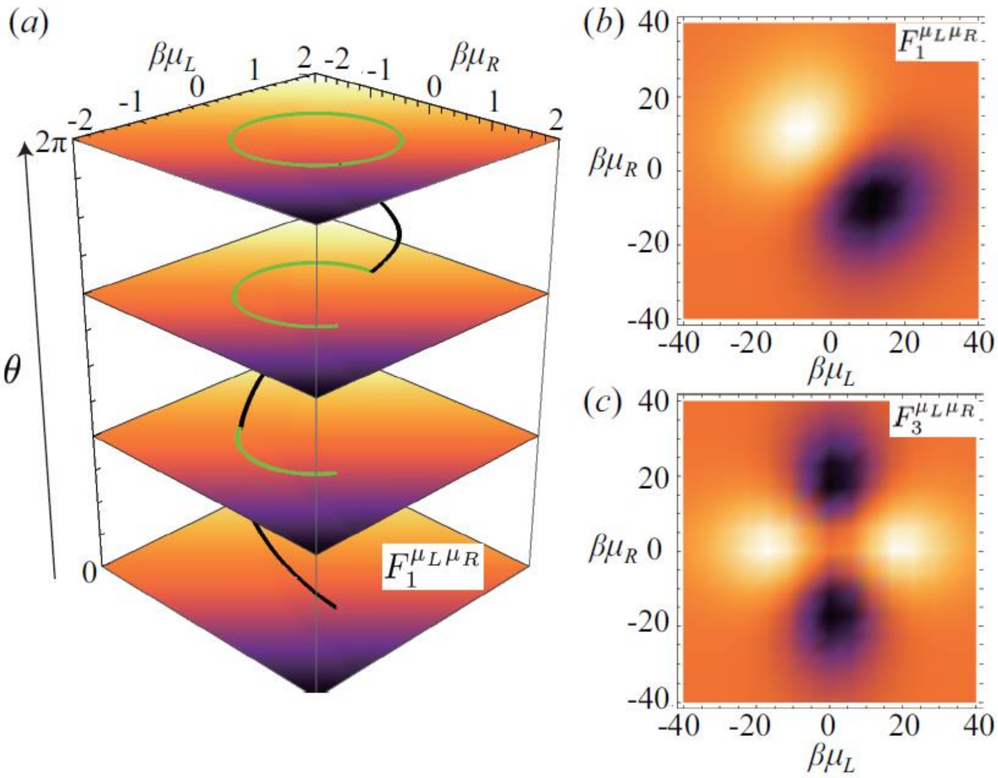
$$\hat{H}^{\mathrm{r}} = \sum_{\alpha,k,\sigma} \epsilon_k \hat{a}^{\dagger}_{\alpha,k,\sigma} \hat{a}_{\alpha,k,\sigma},$$

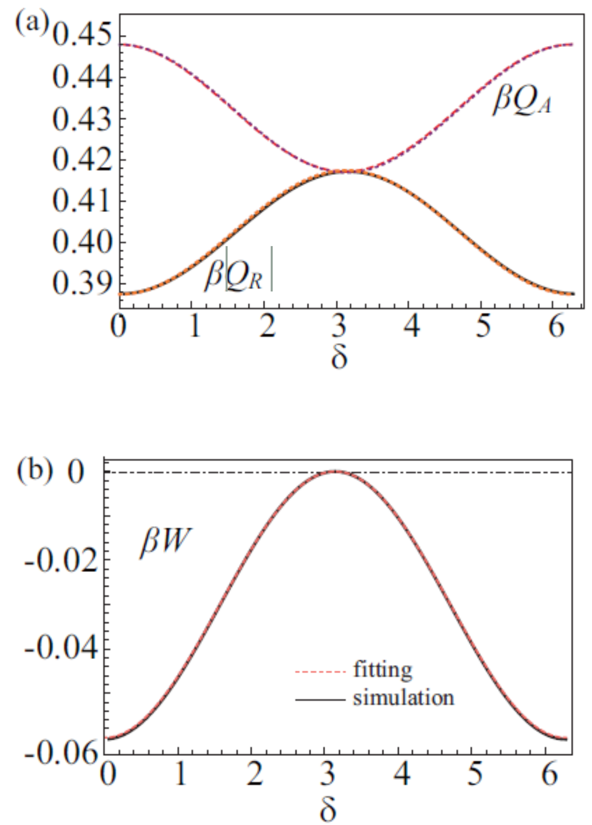
$$\hat{H}^{\mathrm{int}} = \sum_{\alpha.k.\sigma} V_{\alpha} \hat{d}^{\dagger}_{\sigma} \hat{a}_{\alpha,k,\sigma} + \mathrm{h.c.},$$

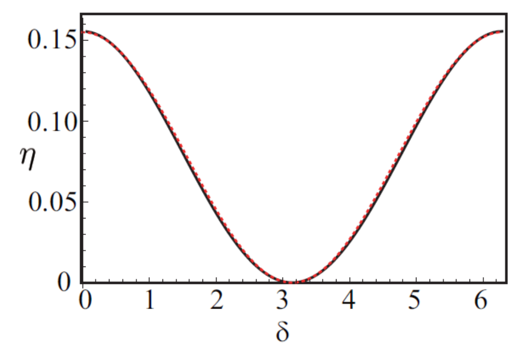
$$U(\theta) := U_0 \lambda(\theta) \qquad \lambda(\theta) := 1 + r_H \sin(\theta + \delta_H)$$

$$\delta_H = \pi/2$$

Thermodynamic results





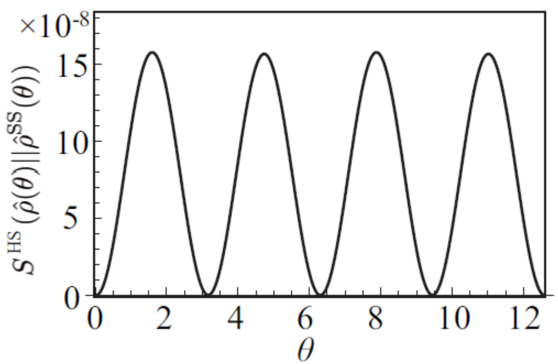


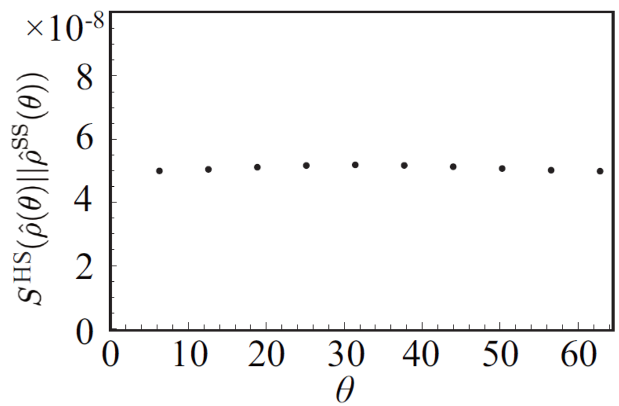
We can extract the work from the engine automatically.

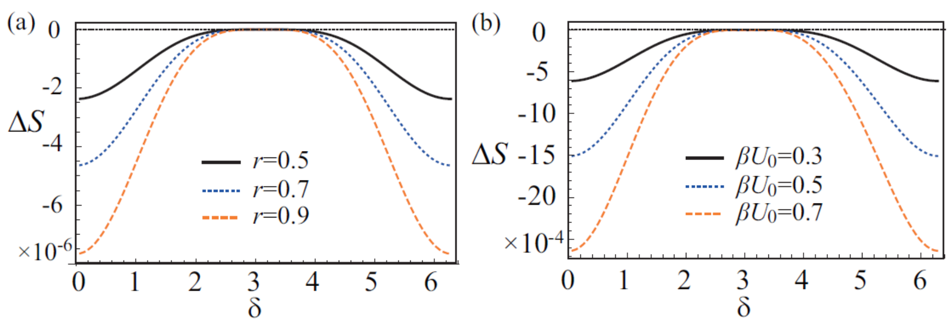
Results of entropy

$|\Delta S|$ is large in the first cycle, but becomes small in the second cycle.

- Entropy changes







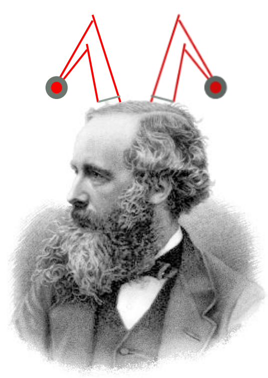
Entropy changes are always negative.

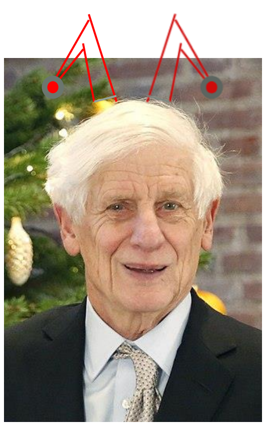
$$\mu_L = \overline{\mu}_L(1 + r_L \sin\theta), \quad \mu_R = \overline{\mu}_R[1 + r_R \sin(\theta + \delta)], \quad \lambda(\theta) := 1 + r_H \sin(\theta + \delta_H)$$

$$\delta_H = \pi/2,\ \bar{\mu} := \overline{\mu_L} = \overline{\mu_R} \text{ and } \bar{r} := r_L = r_R = r_H$$

Conclusion

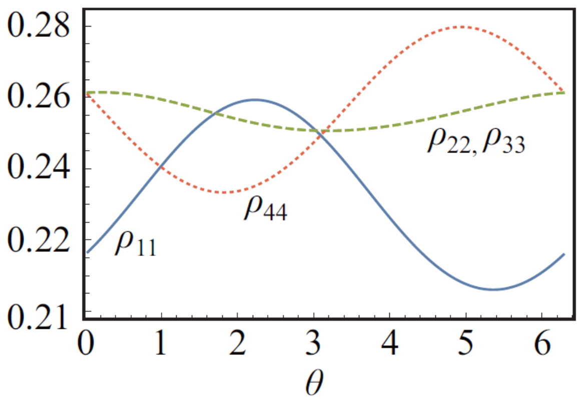
- We implement Maxwell's demon driven by geometrical phase.=>Thouless' demon?
  - The system performs work to external reservoirs.
- The entropy is related to Fisher's information or Hessian matrix around the NESS.
- NESS is the maximum entropy state.
- However, the driven state is deviated from NESS because of the geometrical phase.





KL divergence and relative entropy

- Many documents tell us that these are equivalent.
- However, our analysis indicates that they are different.
- Our relative entropy keeps CPTP but non-monotonic.
  - Completely positivity is related to the positivity of probability.
  - Trace preserving is the conservation of probability.



- KL divergence cannot increase, our relative entropy can increase, because ρ^{SS} does not satisfy the master equation.