GRADUATE SCHOOL
OF CHINA ACADEMY OF
ENGINEERING PHYSICS

CSRC

Geodesic path for the minimal energy cost in shortcuts to isothermality

Geng Li, **Jin-Fu Chen**, C. P. Sun, and Hui Dong

Graduate School of China Academy of Engineering Physics
Beijing Computational Science Research Center

2021/12/16

arXiv: 2110.09137

Content

- Shortcuts to isothermality
- Irreversible work
- Thermodynamic length and optimal protocol
- Conclusion

Shortcuts to adiabacity

Origin Hamiltonian $H_o(t)\,|n(t)\rangle = E_n(t)\,|n(t)\rangle$

Adiabatic approximation

$$|\psi_n(t)\rangle = \exp\left\{-\frac{i}{\hbar}\int_0^t E_n(t')dt' - \int_0^t \langle n(t')|\partial_{t'} n(t')\rangle\, dt'\right\}|n(t)\rangle$$

dynamical Berry

Find $H(t)$ such that $i\hbar\partial_t\,|\psi_n(t)\rangle = H(t)\,|\psi_n(t)\rangle$

The auxiliary Hamiltonian is added as $H(t) = H_o(t) + H_a(t)$

One can boost quantum adiabatic processes in arbitrary finite time.

M. V. Berry, *J. Phys. A: Math. Theor.* **42,** 365303 (2009)

Shortcuts to isothermality

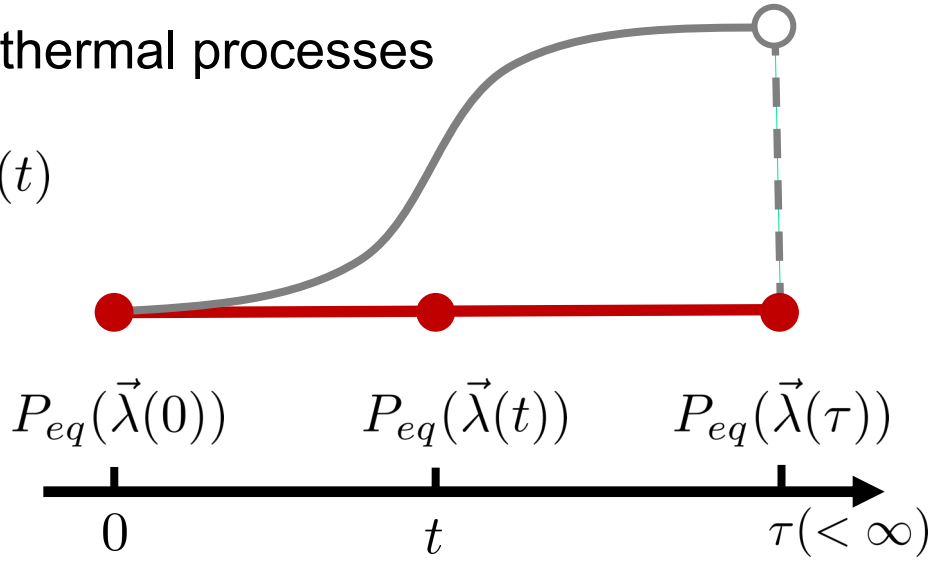
A similar idea can be applied for isothermal processes

Total Hamiltonian $H(t) = H_o(t) + H_a(t)$

Boundary condition $H_a(0) = H_a(\tau) = 0$

Temperature $T = \text{Const}$

$$P_{eq}(\vec{\lambda}(t)) = e^{\frac{1}{T}[F(\vec{\lambda}) - H_o(\vec{\lambda})]}$$



The shortcut control scheme has been constructed for the classical Brownian motion model.

G. Li, H. T. Quan and Z. C. Tu, Phys. Rev. E 96, 012144 (2017).

Dynamics of underdamped Brownian motion

The complete Langevin equation of a single Brownian particle

$$\dot{x}_i = \frac{\partial H}{\partial p_i}$$

$$\dot{p}_i = -\frac{\partial H}{\partial x_i} - \gamma \dot{x}_i + \xi_i(t),$$

Fluctuation-Dissipation relation

$$\langle \xi_i(t)\xi_j(t')\rangle = 2\gamma k_{\mathrm{B}} T \delta_{ij}\delta(t-t')$$

Total Hamiltonian

$$H = H_o + H_a$$

The evolution of the probability distribution $P(\vec{x}, \vec{p}, t)$ is described by the Kramers equation

$$\frac{\partial P}{\partial t} = \sum_i [\underbrace{-\frac{\partial}{\partial x_i}\left(\frac{\partial H}{\partial p_i} P\right) + \frac{\partial}{\partial p_i}\left(\frac{\partial H}{\partial x_i} P}_{\text{deterministic}} + \underbrace{\gamma \frac{\partial H}{\partial p_i} P\right) + \gamma k_{\mathrm{B}} T \frac{\partial^2 P}{\partial p_i^2}}_{\text{dissipation}}]$$

Shortcuts to isothermality

The auxiliary Hamiltonian H_a is employed to realize the shortcut

$$P(\vec{x},\vec{p},t)=P_{eq}(\vec{x},\vec{\lambda})=\mathrm{e}^{\beta[F(\vec{\lambda})-H_o(\vec{x},\vec{p},\vec{\lambda})]} \qquad \beta=\frac{1}{k_{\mathrm{B}}T}$$

Plugging the solution to the Kramers equation, the form of the auxiliary Hamiltonian was found to be

$$H_a(\vec{x},\vec{p},t)=\dot{\vec{\lambda}}\cdot\vec{f}(\vec{x},\vec{p},\vec{\lambda})$$

where $\vec{f}(\vec{x},\vec{p},\vec{\lambda})$ satisfies

$$\sum_i[\frac{\gamma}{\beta}\frac{\partial^2 f_\mu}{\partial p_i^2}-\gamma p_i\frac{\partial f_\mu}{\partial p_i}+\frac{\partial f_\mu}{\partial p_i}\frac{\partial U_{\mathrm{o}}}{\partial x_i}-p_i\frac{\partial f_\mu}{\partial x_i}]=\frac{dF}{d\lambda_\mu}-\frac{\partial U_{\mathrm{o}}}{\partial\lambda_\mu}$$

The explicit expression can be determined with the given potential

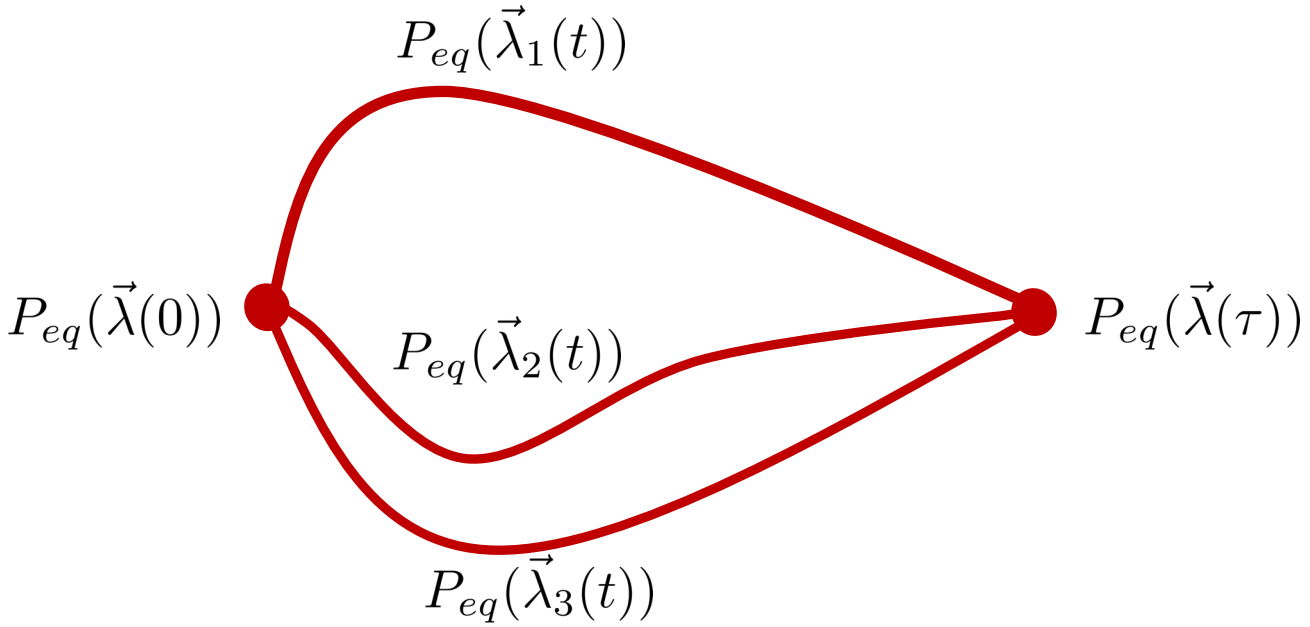
G. Li, H. T. Quan and Z. C. Tu, Phys. Rev. E 96, 012144 (2017).

Content

- Shortcuts to isothermality
- Irreversible work
- Thermodynamic length and optimal protocol
- Conclusion

Irreversible work

Different shortcuts exist for given initial and final states



Which one consume the minimal energy?

Irreversible work

Average work in shortcuts to isothermality

$$W \equiv \left\langle \int_0^\tau dt \frac{\partial H}{\partial t} \right\rangle_{\vec{\xi}} = \underline{\Delta F} + \gamma \sum_i \int_0^\tau dt \iint d\vec{x} d\vec{p} \left(\frac{\partial H_a}{\partial p_i} \right)^2 P_{eq}$$

Free energy difference of initial and final states

Irreversible work

$$W_{irr} \equiv W - \Delta F = \gamma \sum_i \int_0^\tau dt \iint d\vec{x} d\vec{p} \left(\frac{\partial H_a}{\partial p_i} \right)^2 P_{eq}$$

$$= \gamma \sum_i \int_0^\tau dt \left\langle \left(\frac{\partial H_a}{\partial p_i} \right)^2 \right\rangle_{eq} \geq 0$$

$$= \gamma \sum_{\mu\nu i} \int_0^\tau dt \dot{\lambda}_\mu \dot{\lambda}_\nu \left\langle \frac{\partial f_\mu}{\partial p_i} \frac{\partial f_\nu}{\partial p_i} \right\rangle_{eq}$$

Content

- Shortcuts to isothermality
- Irreversible work
- Thermodynamic length and optimal protocol
- Conclusion

Thermodynamic length

Rewrite the irreversible work with the metric

$$W_{irr} = \int_0^\tau \sum_{\mu\nu} \dot{\lambda}_\mu \dot{\lambda}_\nu g_{\mu\nu} dt \qquad g_{\mu\nu} \equiv \gamma \sum_i \left\langle \frac{\partial f_\mu}{\partial p_i} \frac{\partial f_\nu}{\partial p_i} \right\rangle_{eq}$$

Define the thermodynamic length

$$\mathcal{L} = \int_0^\tau dt \sqrt{\sum_{\mu\nu} \dot{\lambda}_\mu \dot{\lambda}_\nu g_{\mu\nu}}$$

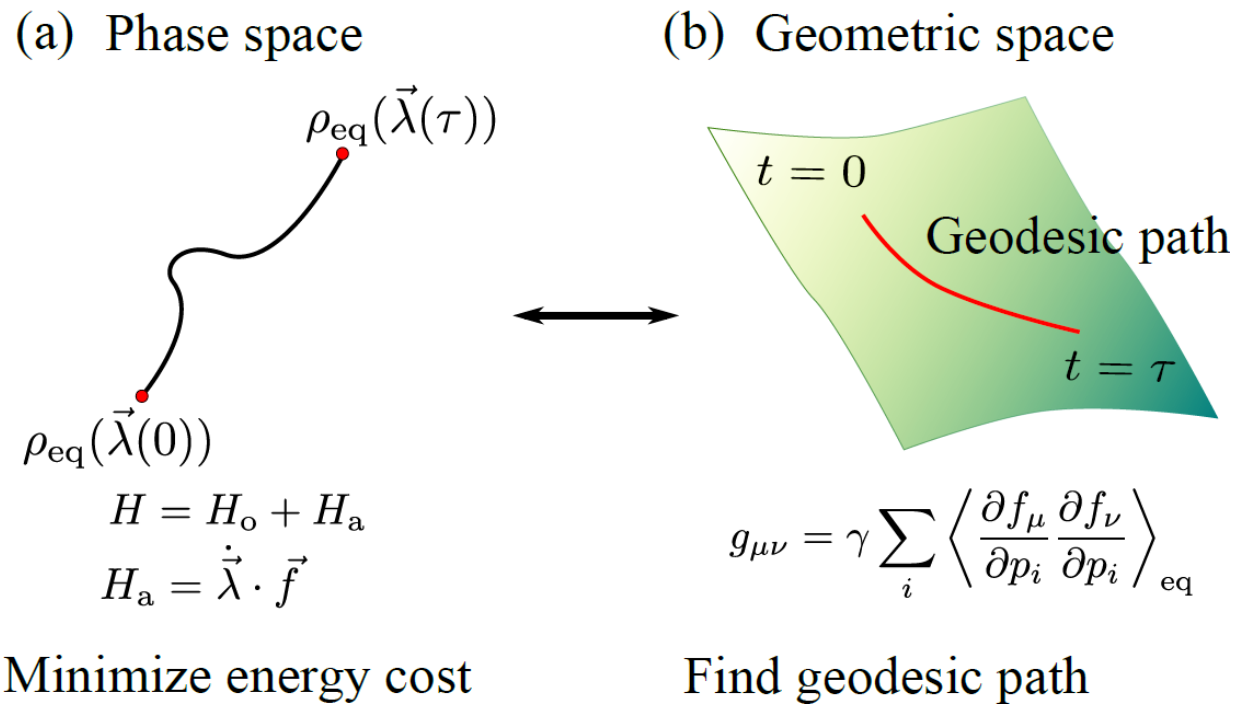
Cauchy-Schwarz inequality leads to

$$W_{irr} \geq \mathcal{L}^2 / \tau$$

The geodesic curve gives the path of the optimal control

$$\ddot{\lambda}_\mu + \sum_{\nu\kappa} \Gamma^\mu_{\nu\kappa} \dot{\lambda}_\nu \dot{\lambda}_\kappa = 0.$$

Thermodynamic length



Some references about thermodynamic length

P. Salamon and R. S. Berry, Phys. Rev. Lett. 51, 1127 (1983).
G. E. Crooks, Phys. Rev. Lett. 99, 100602 (2007).
D. A. Sivak and G. E. Crooks, Phys. Rev. Lett. 108, 190602 (2012).
M. Scandi and M. Perarnau-Llobet, Quantum 3, 197 (2019).
J.-F. Chen, C. P. Sun, and H. Dong, Phys. Rev. E 104, 034117 (2021).

Single control parameter

First example $H_o(x,p,\lambda)=\frac{p^2}{2}+\frac{1}{2}\lambda x^2$

The auxiliary Hamiltonian is $H_a=\frac{\dot{\lambda}}{4\gamma\lambda}\left[(p-\gamma x)^2+\lambda x^2\right]$

Geodesic path $\ddot{\lambda}+\frac{\dot{\lambda}^2}{2g}\frac{\partial g}{\partial\lambda}=0$ Metric $g=\frac{T(\lambda+\gamma^2)}{4\gamma\lambda^3}$

The optimal control with operation time τ is

$$\lambda_{\rm gp}(t)=\frac{\sqrt{1+2\gamma^2(m_s-n_s t/\tau)}+1}{2(m_s-n_s t/\tau)}$$

with

$$m_s=1/\lambda(0)+\gamma^2/(2\lambda(0))$$
$$n_s=1/\lambda(0)+\gamma^2/(2\lambda(0))-1/\lambda(\tau)-\gamma^2/(2\lambda(\tau))$$

The irreversible work is

$$W_{\rm irr}^{\rm min}=\int_0^\tau\dot{\lambda}^2 g dt=n_{\rm s}^2/\tau$$

Two control parameters

Second example $H_o(x,p,\lambda) = \frac{p^2}{2} + \frac{1}{2}\lambda_1 x^2 - \lambda_2 x$

The auxiliary Hamiltonian $H_a = \sum_{\mu=1}^{2} \dot{\lambda}_\mu f_\mu(x,p,\lambda_1,\lambda_1)$

$$f_1 = \frac{(p-\gamma x)^2 + \lambda_1 x^2}{4\gamma\lambda_1} - \frac{\lambda_2 p}{2\lambda_1^2} + (\frac{\gamma\lambda_2}{2\lambda_1^2} - \frac{\lambda_2}{2\gamma\lambda_1})x$$

$$f_2 = \frac{p}{\lambda_1} - \frac{\gamma x}{\lambda_1}$$

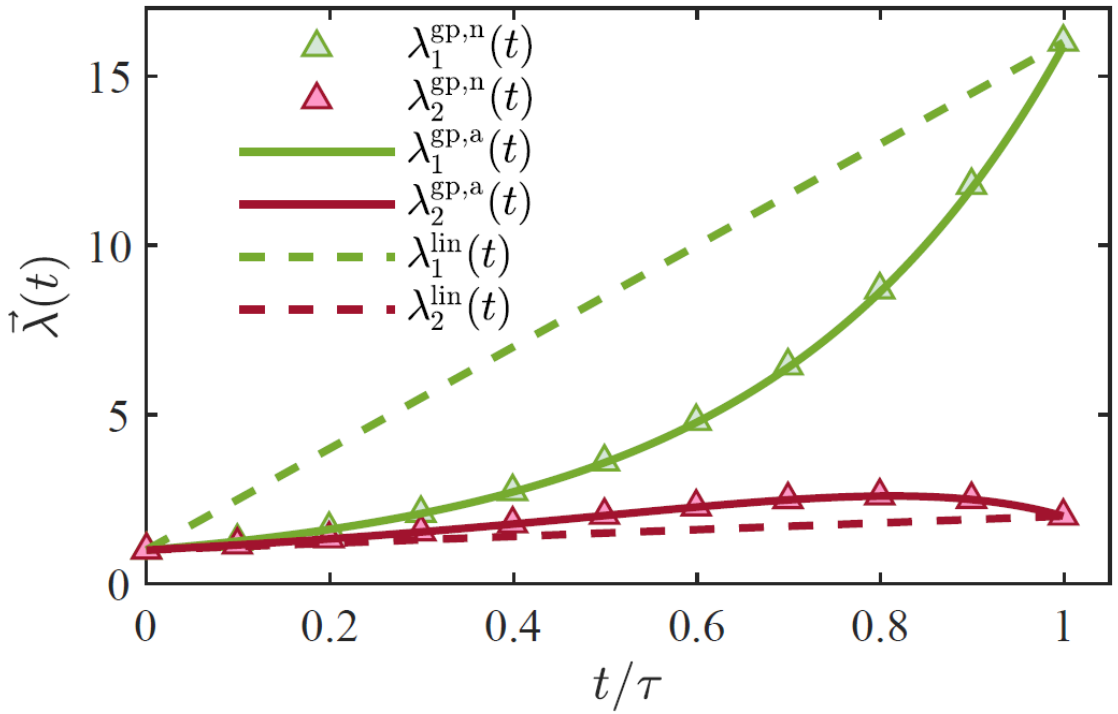
The optimal control is determined by

$$\ddot{\lambda}_1 - \frac{\dot{\lambda}_1^2(3\gamma^2+2\lambda_1)}{2\lambda_1(\gamma^2+\lambda_1)} = 0$$

$$\ddot{\lambda}_2 - \frac{2\dot{\lambda}_1\dot{\lambda}_2}{\lambda_1} + \frac{\dot{\lambda}_1^2\lambda_2(\gamma^2+2\lambda_1)}{2\lambda_1^2(\gamma^2+\lambda_1)} = 0$$

Two control parameters

Comparison between the optimal control and the linear control



$$\vec{\lambda}(0) = (1, 1)$$

$$\vec{\lambda}(\tau) = (16, 2)$$

analytical: $\vec{\lambda}^{\mathrm{gp,a}}$

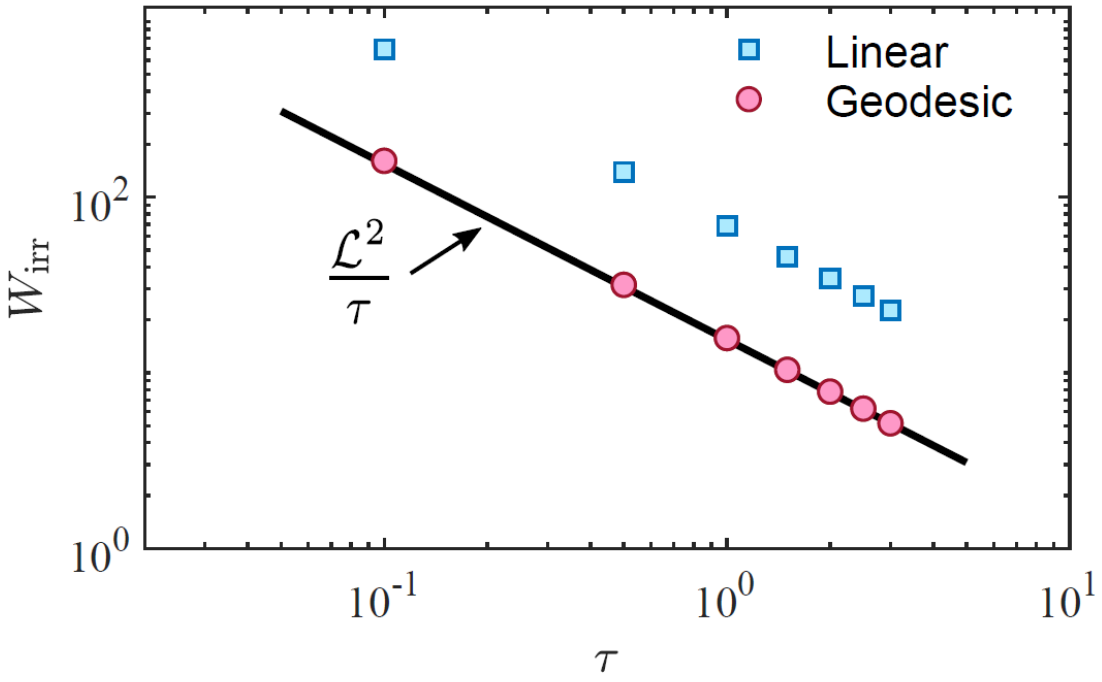
numerical: $\vec{\lambda}^{\mathrm{gp,n}}$

linear control:

$$\vec{\lambda}^{\mathrm{lin}}(t) = [\vec{\lambda}(\tau) - \vec{\lambda}(0)]\frac{t}{\tau} + \vec{\lambda}(0)$$

Two control parameters

The irreversible work in the linear and the optimal controls



The thermodynamic length is given by $\mathcal{L} = \int_0^\tau dt \sum_{\mu\nu} \sqrt{\dot{\lambda}_\mu \dot{\lambda}_\nu g_{\mu\nu}}$

Conclusion

- A geometric approach to find the optimal control via shortcut to isothermality.
- The irreversible work is bounded by the thermodynamic length.
- The strict $1/\tau$ scaling of the irreversible work for the Brownian motion model.



Thank You