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Kim Memoial Hall, POSTECH

Path integral approach to quantum heat

Haitao Quan (Peking University)

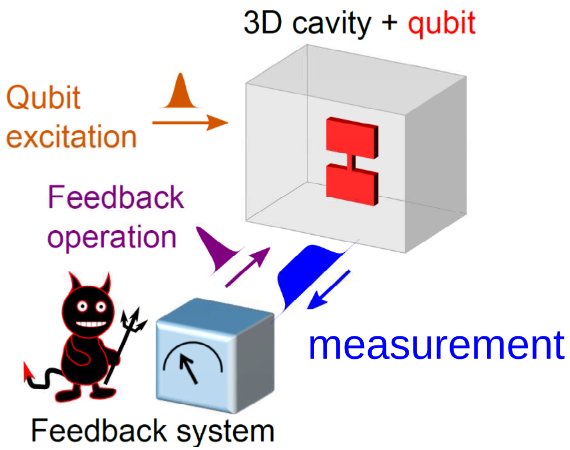
in collaboration with:

Ken Funo (Currently in RIKEN, Japan)

based on K. Funo and H. T. Quan *PRE, 98, 012113 (2018)*
K. Funo and H. T. Quan *PRL, 121, 040602 (2018)*

Outline

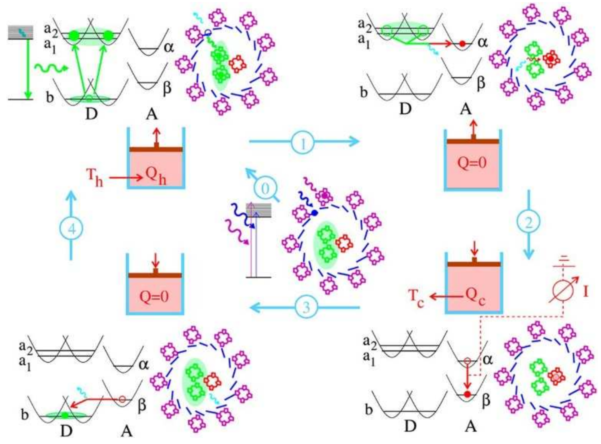
- Background and motivation
- Trajectory heat along every pair of Feynman paths
- Microscopic reversibility and Jarzynski equality
- Quantum-classical correspondence of trajectory heat and heat statistics
- Summary



Maxwell's demon

Y. Masuyama, *et al.*, arXiv:1709.00548

nonequilibrium statistical mechanics



light-harvesting cycles

P. Nalbach, M. Thorwart PNAS **110,** 2693 (2013)

quantum thermodynamics

quantum information theory

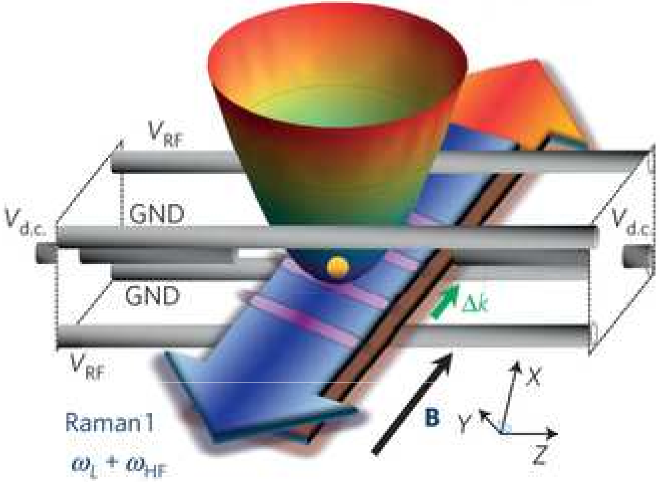
quantum information processing technologies

nanoscopic physics

bio physics

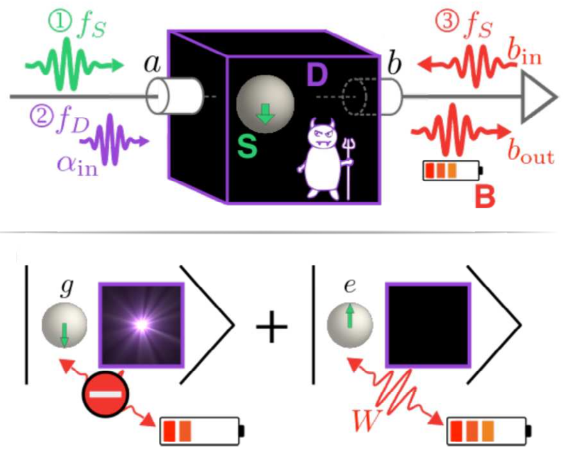
quantum thermodynamics: recent experiments

Trapped ions



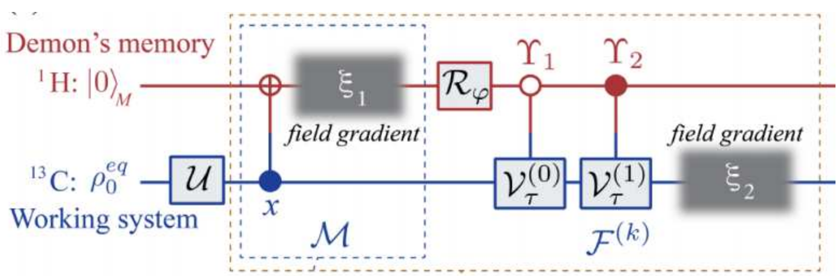
S. An, *et al.*, Nat. Phys. **11,** 193 (2015)

Circuit QED

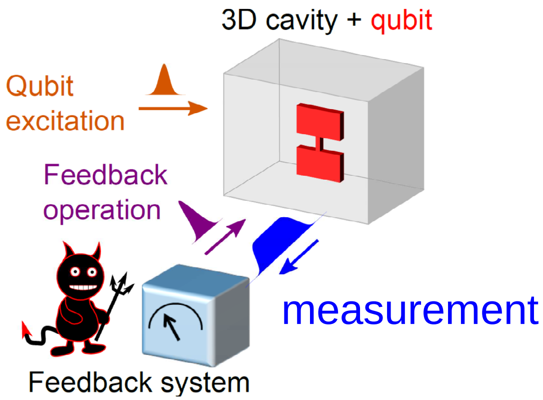


N. Cottet, *et al.*, *PNAS* **114,** 7561 (2017)

NMR



P. A. Camati *et al.*, PRL **117**, 240502 (2016)



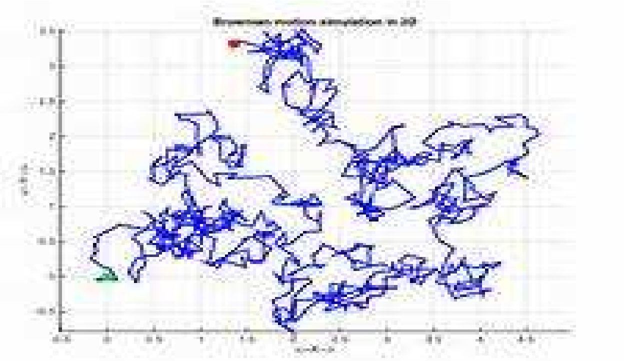
Y. Masuyama, *et al.*, arXiv:1709.00548

Trajectory work and heat in classical stochastic systems

Work, heat and Entropy as functionals of a trajectory

Work: $dw = \frac{\partial H_\lambda(x(t))}{\partial \lambda} \dot{\lambda}\, dt$ Heat: $dq = \frac{\partial H_\lambda(x(t))}{\partial x} \dot{x}\, dt$

C. Jarzynski, Phys. Rev. Lett 78, 2690 (1997)
K. Sekimoto, J. Phys. Soc. Jap. 66, 1234 (1997)



For overdamped Langevin Dynamics

$$\dot{x} = \mu F(x,\lambda) + \zeta = \mu[-\partial_x V(x,\lambda) + f(\lambda)] + \zeta,$$

$$\langle \zeta(\tau)\zeta(\tau')\rangle = 2D\delta(\tau - \tau')$$

Heat: $dq = (1/\mu)(\dot{x} - \zeta)dx$

Work: $dw = f dx + \partial_\lambda V(x,\lambda) d\lambda$

Ken Sekimoto, Stochastic Energetics (2010)

Feynman path approach to quantum trajectory work

- Work functional is defined along individual path, (Feynman)
- It is deeper than the two-point measurement method. (Schrodinger)

✓ quantum corrections to the classical work funcitonal

$$W_\nu[x] = W_{cl}[x] + \frac{i\nu}{2} W_q^{(1)}[x] + \frac{(i\nu)^2}{3!} W_q^{(2)}[x] + \cdots$$

✓ quantum-classical correspondence of the work statistics

K. Funo and H. T. Quan *PRL, 121, 040602 (2018)*

C. Aron, G. Biroli, and L. F. Cugliandolo, *SciPost*, 4, 008 (2018)

J. Yeo, *arXiv*: 1909.08212

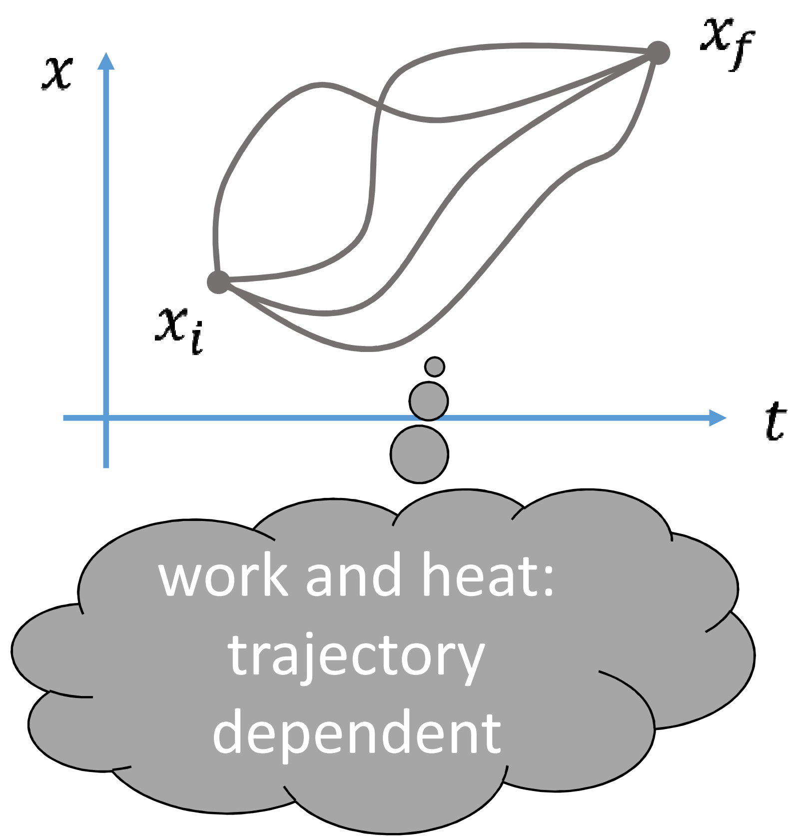
How about trajectory heat?

- Trajectory heat is more subtle than trajectory work

- Even in classical systems, the strong coupling regime is not well understood

- We restrict to weak coupling regime

- We study quantum Brownian motion



P. Talkner, P. Hanggi, *PRE, 94, 022143 (2016)*
Open system trajectories specify fluctuating work but not heat

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- Background and motivation

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Quantum Brownian motion – Caldeira Leggett model

- Composite system (system + bath)

$$H_{tot}(\lambda_t) = H_S(\lambda_t) + H_{SB} + H_B$$

system Hamiltonian

$$H_S(\lambda_t) = \frac{\hat{p}^2}{2M} + V(\lambda_t, \hat{x})$$

counter term

interaction Hamiltonian

$$H_{SB} = -\hat{x} \otimes \sum_k c_k \hat{q}_k + \sum_k \frac{c_k^2 \hat{x}^2}{2m_k \omega_k^2}$$

bath Hamiltonian

$$H_B = \sum_k \left(\frac{\hat{p}_k^2}{2m_k} + \frac{m_k \omega_k^2}{2} \hat{q}_k^2\right)$$

Quantum Brownian motion – Caldeira Leggett model

- ✓ semi-classical limit $\rightarrow$ underdamped Fokker-Planck equation

A. O. Caldeira and A. J. Leggett, Physica A **121,** 587 (1983)

- ✓ non-Markovian, non-rotating wave,

- ✓ exactly solvable (spin-boson, HPZ master equation)
  & various calculation methods

B. L. Hu, J.P. Paz, Y. Zhang, PRD **45,** 2843 (1992)
Y. Tanimura, J. Phys. Soc. Jpn. **75,** 082001 (2006)

- ✓ path integral method to study the reduced dynamics

C. Morais Smith and A. O. Caldeira, PRA **36,** 3509 (1987)
H. Grabert, P. Schramm, and G.-L. Ingold, Phys. Rep. **168,** 115 (1988)

Definition of the heat probability distribution

- Two-point energy measurements

final energy

$$Q_{m,m'} = E_m^B - E_{m'}^B$$

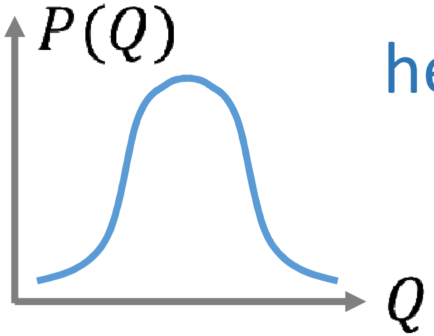
initial energy

initial probability

$$p^B(m) = e^{-\beta E_m^B}/Z^B$$

transition probability

$$P(m' \leftarrow m) = \mathrm{Tr}_S\left[\langle E_{m'}^B | U_{SB} | E_m^B \rangle \rho^S(0) \langle E_m^B | U_{SB} | E_{m'}^B \rangle\right]$$



heat probability distribution

$$P(Q) = \sum_{m,m'} \delta\left(Q - Q_{m,m'}\right) P(m' \leftarrow m) p^B(m)$$

Characteristic function of heat

Fourier transformation: $\chi_Q(\nu) = \int dQ e^{i\nu Q} P(Q)$

characteristic function of heat

$$\chi_Q(\nu) = \mathrm{Tr}[U_{SB} e^{i\nu H_B} \rho_{SB}(0) U_{SB}^{\dagger} e^{-i\nu H_B}]$$

✓ first moment = average heat:

$$\langle Q \rangle = -i\partial_\nu \chi_Q(\nu)\Big|_{\nu=0} = \mathrm{Tr}[H_B \rho_B(0)] - \mathrm{Tr}[H_B \rho_B(\tau)]$$

✓ n-th moment: $\langle Q^n \rangle = (-i)^n \partial_\nu^n \chi_Q(\nu)|_{\nu=0}$

Path integral method

- initial state: $\rho_{SB}(0) = \rho_S(0) \otimes \frac{e^{-\beta H_B}}{Z_B}$

density matrix at time τ:

unitary dynamics

$$\langle x_f|\rho_s(\tau)|y_f\rangle = \int dx_i dy_i \int DxDy\, e^{\frac{i}{\hbar}(S[x]-S[y])} F_{FV}[x,y]\rho_S(x_i,y_i)$$

nonunitary dynamics
(environmental effect)

- action: $S[x] = \int_0^\tau dt(\frac{M}{2}\dot{x}^2(t) - V[\lambda_t, x(t)])$

- Feynman-Vernon influence functional

$$F_{FV}[x,y] = \exp\left[+\frac{1}{\hbar}\int dt\, ds\, \underline{L(s-t)}x(t)y(s) - \frac{1}{\hbar}\int dtds\,\{L(t-s)x(t)x(s) + L^*(t-s)y(t)y(s)\} + \text{counterterm}\right]$$

bath correlation function

$x(t)$: forward path
$y(s)$: backward path

Path integral expression of heat statistics

characteristic function of heat

$$\chi_Q(\nu) = \mathrm{Tr}[U_{SB} e^{i\nu H_B} \rho_{SB}(0) U_{SB}^{\dagger} e^{-i\nu H_B}]$$

path integral expression

$$\chi_Q(\nu) = \int dx_f dy_f dx_i dy_i \delta(x_f - y_f) \int DxDy\, \underbrace{e^{\frac{i}{\hbar}(S[x]-S[y])} F_{FV}[x,y] \rho_S(x_i, y_i)}_{\text{time-evolution}} e^{i\nu Q_\nu[x,y]}$$

heat functional

$$Q_\nu[x,y] = -\frac{i}{\hbar\nu} \int dtds\big(L(s-t+\hbar\nu) - L(s-t)\big)x(t)y(s)$$

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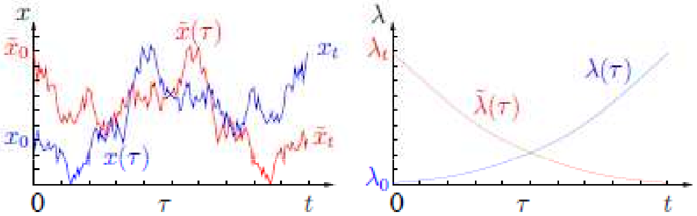
Microscopic reversibility in classical Brownian motion

- Path integral representation
  - "Boltzmann factor for a whole trajectory"

$$p[\zeta(\tau)] \sim \exp\ [-\int_0^t d\tau\ \zeta^2(\tau)/4D]$$

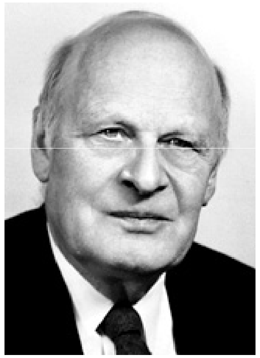
$$p[x(\tau)|x_0] \sim \exp\ [-\int_0^t d\tau\ (\dot{x}-\mu F)^2/4D]$$



  - "time reversal" $\tilde{x}(\tau) \equiv x(t-\tau)$ and $\tilde{\lambda}(\tau) \equiv \lambda(t-\tau)$
  - Ratio of forward to reversed path

$$\frac{p[x(\tau)|x_0]}{\tilde{p}[\tilde{x}(\tau)|\tilde{x}_0]} = \frac{\exp\ [-\int_0^t d\tau\ (\dot{x}-\mu F)^2/4D]}{\exp\ [-\int_0^t d\tau\ (\dot{\tilde{x}}-\mu \tilde{F})^2/4D]}$$

$$= \exp\ \beta \int_0^t d\tau\ \dot{x}F = \exp\ \beta q[x(\tau)] = \exp \Delta s_m$$



Lars Onsager

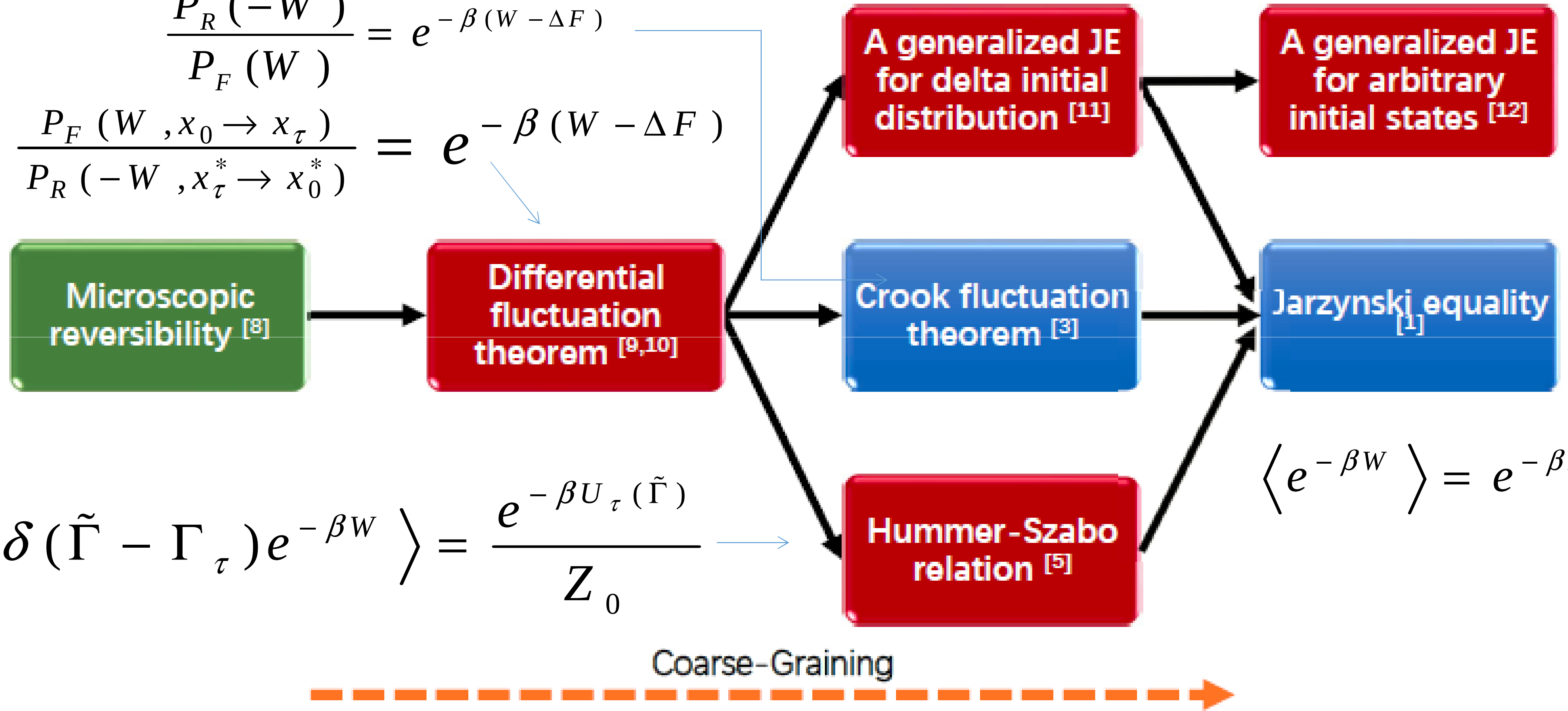
L. Onsager, S. Machlup, Phys. Rev. 91, 1505 (1953).

All nonequilibrium work fluctuation theorems can be derived from this relation!

Hierarchy of fluctuation theorems

$$\frac{P_R(-W)}{P_F(W)} = e^{-\beta(W-\Delta F)}$$

$$\frac{P_F(W, x_0 \to x_\tau)}{P_R(-W, x_\tau^* \to x_0^*)} = e^{-\beta(W-\Delta F)}$$



$$\left\langle e^{-\beta W} \right\rangle = e^{-\beta \Delta F}$$

$$\left\langle \delta(\tilde{\Gamma} - \Gamma_\tau) e^{-\beta W} \right\rangle = \frac{e^{-\beta U_\tau(\tilde{\Gamma})}}{Z_0}$$

T. M. Hoang, ..., H. T. Quan, and T. Li, Phys. Rev. Lett 120, 080602 (2018)

Microscopic reversibility in quantum Brownian motion

heat functional ($\nu = -i\beta$)

$$Q_\beta[x,y] = -\frac{1}{\hbar\beta}\int dtds\big(L(t-s)-L(s-t)\big)x(t)y(s)$$

microscopic reversibility

$$\frac{\tilde{\mathcal{P}}\left[\tilde{x}(\tilde{t}),\tilde{y}(\tilde{s})\middle|x_f,y_f\right]}{\mathcal{P}[x(t),y(s)|x_i,y_i]} = e^{\beta Q_\beta[x,y]}$$

conditional path probability distribution

density matrix at time τ:

$$\langle x_f|\rho_s(\tau)|y_f\rangle = \int dx_i dy_i \int DxDy\, \overbrace{e^{\frac{i}{\hbar}(S[x]-S[y])}F_{FV}[x,y]}^{\mathcal{P}[x(t),y(s)|x_i,y_i]}\rho_S(x_i,y_i)$$

Asymmetric part of the influence functional

- Forward path

$$e^{\frac{i}{\hbar}(S[x]-S[y])}F_{FV}[x,y]$$

$$= \exp\left[+\frac{1}{\hbar}\int dt\,ds\,L(s-t)x(t)y(s)\right.$$

$$-\frac{1}{\hbar}\int dtds\,L(t-s)x(t)x(s)$$

$$-\frac{1}{\hbar}\int dtds\,L^*(t-s)y(t)y(s)$$

$$\left.+\frac{i}{\hbar}(S[x]-S[y])+\mathrm{c.t.}\right]$$

- Backward path

$$\tilde{t}=\tau-t,\tilde{x}(\tilde{t})=x(t),\tilde{\lambda}_{\tilde{t}}=\lambda_t$$

$$e^{\frac{i}{\hbar}(\tilde{S}[\tilde{x}]-\tilde{S}[\tilde{y}])}\tilde{F}_{FV}[\tilde{x},\tilde{y}]$$

$$= \exp\left[+\frac{1}{\hbar}\int d\tilde{t}\,d\tilde{s}\,L(\tilde{s}-\tilde{t})\tilde{x}(\tilde{t})\tilde{y}(\tilde{s})\right.$$

$$-\frac{1}{\hbar}\int d\tilde{t}d\tilde{s}\,L(\tilde{t}-\tilde{s})x(\tilde{t})x(\tilde{s})$$

$$-\frac{1}{\hbar}\int d\tilde{t}d\tilde{s}\,L^*(\tilde{t}-\tilde{s})\tilde{y}(\tilde{t})\tilde{y}(\tilde{s})$$

$$\left.+\frac{i}{\hbar}(\tilde{S}[\tilde{x}]-\tilde{S}[\tilde{y}])+\mathrm{c.t.}\right]$$

related to the heat functional

$\neq$

time asymmetric

$=$

time symmetric

Asymmetric part of the influence functional

- Forward path

$$e^{\frac{i}{\hbar}(S[x]-S[y])}F_{FV}[x,y]$$

$$= \exp\left[+\frac{1}{\hbar}\int dt\, ds\, L(s-t)x(t)y(s)\right]$$

- Backward path

$$\tilde{t} = \tau - t, \tilde{x}(\tilde{t}) = x(t), \tilde{\lambda}_{\tilde{t}} = \lambda_t$$

$$e^{\frac{i}{\hbar}(\tilde{S}[\tilde{x}]-\tilde{S}[\tilde{y}])}\tilde{F}_{FV}[\tilde{x},\tilde{y}]$$

$$\neq \quad = \exp\left[+\frac{1}{\hbar}\int d\tilde{t}\, d\tilde{s}\, L(\tilde{s}-\tilde{t})\tilde{x}(\tilde{t})\tilde{y}(\tilde{s})\right]$$

time asymmetric

$$= +\frac{1}{\hbar}\int dt\, ds\, L(t-s)x(t)y(s)$$

heat functional $(\nu = -i\beta)$

$$Q_\beta[x,y] = \frac{1}{\hbar\beta}\int dtds\big(L(t-s) - L(s-t)\big)x(t)y(s)$$

Microscopic reversibility

- heat functional satisfies the microscopic reversibility

$$\frac{\tilde{\mathcal{P}}\left[\tilde{x}(\tilde{t}),\tilde{y}(\tilde{s})\middle|x_f,y_f\right]}{\mathcal{P}[x(t),y(s)|x_i,y_i]} = e^{\beta Q_\beta[x,y]}$$

- when there is no heat bath, influence functional equals to 1, heat vanishes
- heat functional as a measure of time-asymmetry along Feynman paths
- key relation for showing fluctuation theorems and Jarzynski's equality

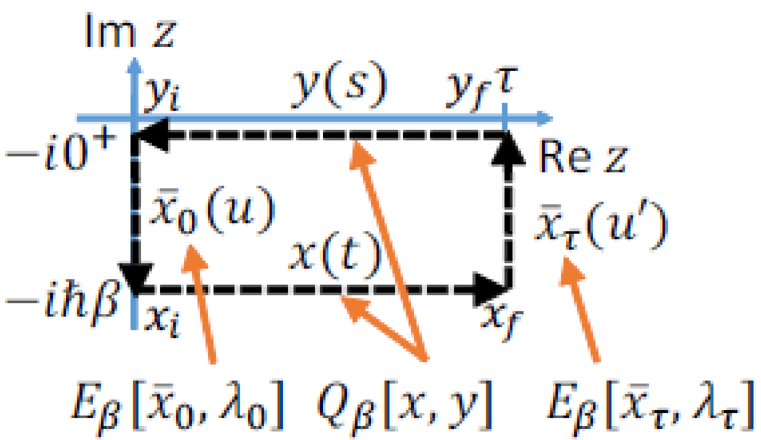
K. Funo and H. T. Quan *PRE, 98, 012113 (2018)*

Definition of the internal energy functional

- initial state: canonical distribution [imaginary path integral]

$$\langle x_i|\rho_s(0)|y_i\rangle = \frac{1}{Z_S(\lambda_0)}\int D\bar{x}_0\, e^{-\frac{1}{\hbar}S^{(\mathrm{E})}[\bar{x}_0,\lambda_0]}$$

initial energy functional



$$E_\beta[\bar{x}_0,\lambda_0] = \frac{1}{\hbar\beta}S^E[\bar{x}_0,\lambda_0]$$

classical limit

$$\longrightarrow \frac{M}{2}[\dot{\bar{x}}_0]^2 + V[\bar{x}_0,\lambda_0] + O(\hbar)$$

K. Funo and H. T. Quan *PRE, 98, 012113 (2018)*

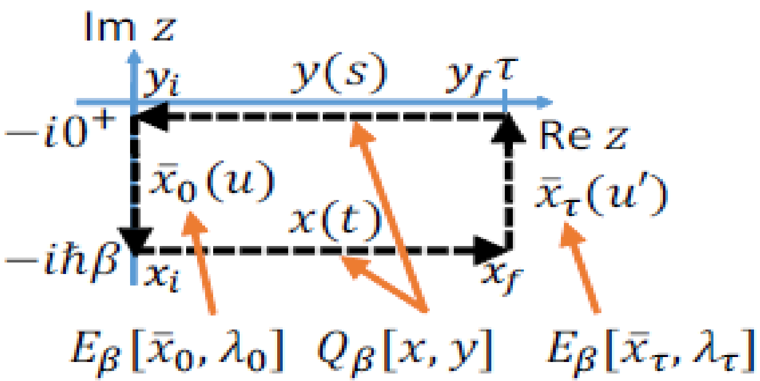
Detailed fluctuation theorem and Jarzynski's equality

- definition of work (weak coupling)

$$W_\beta[\bar{x}_0, x, y, \bar{x}_\tau] = E_\beta[\bar{x}_\tau, \lambda_\tau] - E_\beta[\bar{x}_0, \lambda_0] - Q_\beta[x, y]$$

- detailed fluctuation theorem

$$\frac{\tilde{\mathcal{P}}\left[\tilde{x}(\tilde{t}), \tilde{y}(\tilde{s}) \middle| x_f, y_f\right] e^{-\frac{1}{\hbar} S^E[\bar{x}_\tau, \lambda_\tau]} / Z_S(\lambda_\tau)}{\mathcal{P}[x(t), y(s) | x_i, y_i] e^{-\frac{1}{\hbar} S^E[\bar{x}_0, \lambda_0]} / Z_S(\lambda_0)} = e^{-\beta(W_\beta[\bar{x}_0, x, y, \bar{x}_\tau] - \Delta F)}$$



- Jarzynski's equality

$$\left\langle e^{-\beta(W_\beta - \Delta F)} \right\rangle_{\mathbf{q-path}} = 1$$

K. Funo and H. T. Quan *PRE, 98, 012113 (2018)*

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Properties of the heat functional: classical limit

Trajectory heat

$$Q_\nu[x,y] = -\frac{i}{\hbar\nu}\int dtds\big(L(s-t+\hbar\nu) - L(s-t)\big)x(t)y(s)$$

classical limit

Ohmic spectrum

Weak coupling strength

$$\longrightarrow Q_{\mathrm{cl}}[X,\Omega] = -\frac{\gamma}{M}\int dt\, P^2(t) + \int dt\,\frac{P(t)}{M}\Omega(t) + O(\hbar)$$

Sekimoto (1998)

heat statistics

$$\chi_Q(\nu) \to \langle e^{i\nu Q_{\mathrm{cl}}}\rangle_{\mathrm{cl-path}}$$

✓ Quantum-classical correspondence

Summary

•We define trajectory heat along every pair of Feynman paths, and find the first law of thermodynamics along Feynman paths

•The microscopic reversibility can be proven for the quantum Brownian motion (Caldeira-Leggett model)

•Jarzynski equality in quantum Brownian motion model can be formulated based on the trajectory heat along Feynman paths

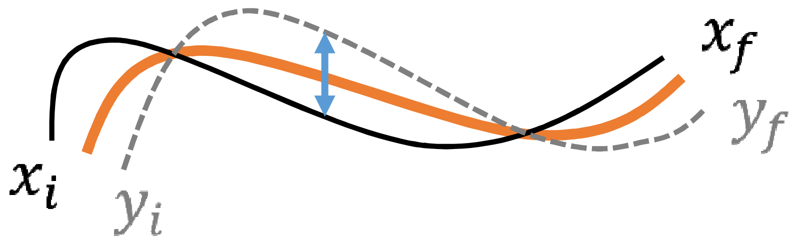
•Correspondence between quantum trajectory heat and classical trajectory heat are established in this model

Thank you!

Classical coordinate and thermal noise from the Caldeira-Leggett model

forward coordinate $x(t)$

backward coordinate $y(t)$



center coordinate $\quad X(t) = \frac{x(t)+y(t)}{2} \overset{\hbar \to 0}{\longrightarrow}$ classical coordinate

quantum fluctuations $\quad \xi(t) = x(t) - y(t)$

thermal noise $\quad \Omega(t) = i \int_0^\tau ds\, \Re[L(t-s)]\xi(s)$

(properties are discussed later)

Classical limit of the trajectory heat

Trajectory heat

$$Q_\nu[x,y] = -\frac{i}{\hbar\nu}\int dtds\big(L(s-t+\hbar\nu) - L(s-t)\big)x(t)y(s)$$

$$= -i\int dtds\dot{L}(s-t)x(t)y(s) + O(\hbar\nu)$$

$$= Q_{\mathrm{cl}}[X,\Omega] + \cancel{Q_{\mathrm{int}}[X,\Omega]} + \cancel{Q_{\mathrm{slip}}[X,\Omega]} + O(\hbar\nu)$$

weak coupling

interaction energy ΔH_{SB}

initial state ≠ conditional thermal state of B

$$p_{SB}(0) \neq p_S(x)e^{-\beta(H_B+H_{SB})}/Z_B$$

Classical limit of the trajectory heat

heat functional

$$Q_\nu[x,y] = -\frac{i}{\hbar\nu}\int dtds\big(L(s-t+\hbar\nu) - L(s-t)\big)x(t)y(s)$$

$$= -i\int dtds\dot{L}(s-t)x(t)y(s) + O(\hbar\nu)$$

$$= Q_{\mathrm{cl}}[X,\Omega] + \cancel{Q_{\mathrm{int}}[X,\Omega]} + \cancel{Q_{\mathrm{slip}}[X,\Omega]} + O(\hbar\nu)$$

weak coupling

classical fluctuating heat (non-Markovian)

$$Q_{\mathrm{cl}}[X,\Omega] = \int dt\,\dot{X}(t)(\Omega(t) - \int ds\,K(t-s)\dot{X}(s))$$

$$\xrightarrow{\text{Ohmic spectrum}} Q_{\mathrm{cl}}[X,\Omega] = -\frac{\gamma}{M}\int dt\,P^2(t) + \int dt\,\frac{P(t)}{M}\Omega(t)$$

Sekimoto (1998)

Classical limit of the Caldeira-Leggett model

$\hbar$ expansion for the action:

$$\frac{i}{\hbar}(S[x]-S[y]) = -\frac{i}{\hbar}\int dt\, \xi(t)\left(M\ddot{X}(t)+V'(X)\right) - \frac{i}{\hbar}M\xi_i\dot{X}_i + O(\xi^3)$$

Feynman-Vernon influence functional:

$$F_{FV}[x,y]$$
$$= \exp\left[\frac{i}{\hbar}\int dt\,\xi(t)\left(\Omega(t) - \int ds\,\underline{K(t-s)}\dot{X}(s)\right) - \frac{i}{\hbar}X_i\int dt\,K(t)\xi(t)\right]$$

classical bath correlation function

c.f. Ohmic spectrum

$K(t-s) = 2M\gamma\delta(t-s)$

thermal noise via Stratonovich-Hubbard transformation

$$\langle\Omega(t)\rangle = 0, \quad \langle\Omega(t)\Omega(s)\rangle = \hbar\Re[L(t-s)] = \beta^{-1}K(t-s) + O(\hbar\beta)$$

Classical limit of the characteristic function of heat

characteristic function of heat

$$\chi_Q(\nu) = \int dx_f dy_f dx_i dy_i \delta(x_f - y_f) \int DxDy\, e^{\frac{i}{\hbar}(S[x]-S[y])} F_{FV}[x,y] \rho_S(x_i, y_i) e^{i\nu Q_\nu[x,y]}$$

$$= \int dX_f dX_i \int DXD\xi D\Omega\, P[\Omega] \exp\left[-\frac{i}{\hbar} \int dt\, \xi(t) \left(M\ddot{X}(t) + V'(X) + \int ds\, K(t-s)\dot{X}(s) - \Omega(t) + X_i \int dt\, K(t) \right) \right] \rho_S(X_i, \dot{X}_i) e^{i\nu Q_{\mathrm{cl}}[x,y]} + O(\hbar)$$

Wigner function

$$= \int dX_f dX_i \int DXD\Omega\, P[\Omega] \underline{\delta(M[X,\Omega])}\, \rho_S(X_i, \dot{X}_i) e^{i\nu Q_{\mathrm{cl}}[x,y]}$$

classical trajectory satisfying non-Markovian Langevin equation

$$M[X,\Omega] = M\ddot{X}(t) + V'(X) + \int ds\, K(t-s)\dot{X}(s) - \Omega(t) + X_i \int dt\, K(t) = 0$$

Classical limit of the characteristic function of heat

characteristic function of heat

$$\chi_Q(\nu) \to \left\langle e^{i\nu Q_{\mathrm{cl}}[x,y]} \right\rangle_{\mathrm{cl-path}}$$

quantum-classical correspondence principle of the heat statistics