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Quantum Stochastic Thermodynamics for a Simple Floquet System

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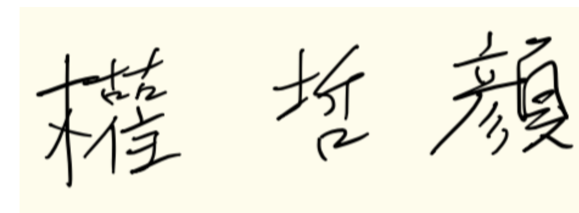

0. **Motivation**
I. **Introduction**
II. **A simple Floquet system**
III. **Time evolution**
IV. **Fluctuation theorem**
V. **Summary**

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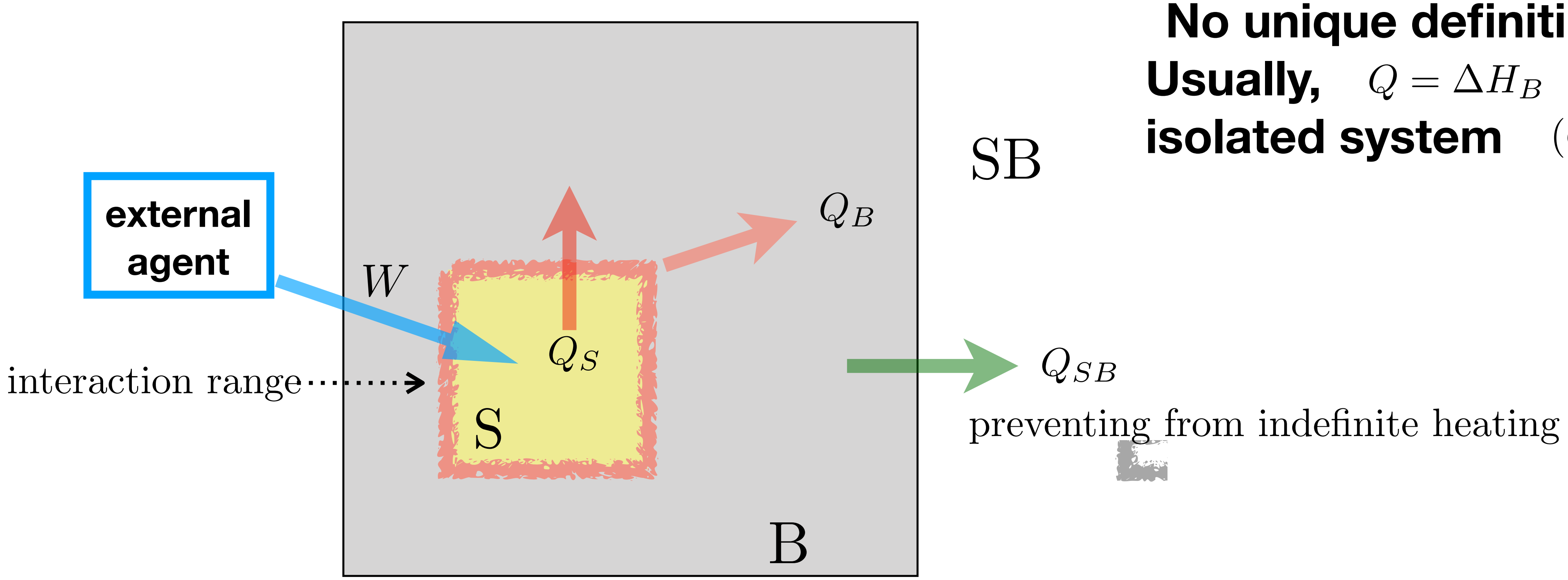
0. Motivation

1. **Nonequilibrium quantum thermodynamics**
   - Time-dependent Hamiltonian should be considered.

2. **Strong coupling view**



No unique definition of heat.
Usually, $Q = \Delta H_B$ **is used for isolated system** $(Q_{SB} = 0)$

First laws $\Delta H_S = W - Q_S \quad \Delta H_B = Q_B - Q_{SB} \quad \Delta H_{tot} = \Delta H_S + \Delta H_B + \Delta H_I = W - Q_{SB}$

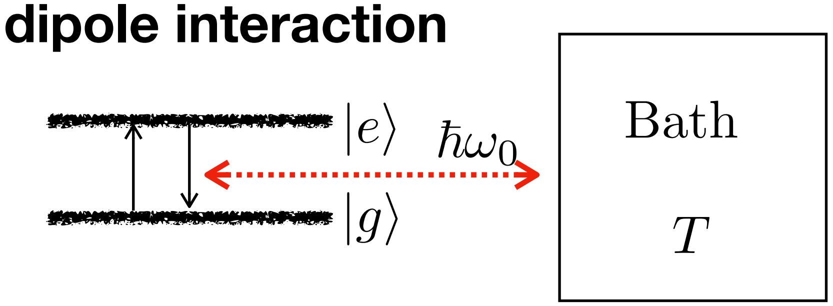
$\longrightarrow \quad \Delta H_I = Q_S - Q_B$

3. **System point of view in terms of measurable quantities** $W, \; Q_S, \; \rho_S$
   - No relevant quantum master equation (Lindblad eq) for time-dependent protocol except special cases included by this talk

I. Introduction

based on *The theory of open quantum systems*, Breuer and Petruccione, Oxford, 2002

1. A two-level system weakly coupled to optical bath via dipole interaction



$$H_0 = \frac{\hbar\omega_0}{2}\sigma_3$$

$$\sigma_1 = |e\rangle\langle g| + |g\rangle\langle e|,\ \ \sigma_2 = -i(|e\rangle\langle g| - |g\rangle\langle e|),\ \ \sigma_3 = |e\rangle\langle e| - |g\rangle\langle g|$$

$$\sigma_+ = \frac{1}{2}(\sigma_1 + i\sigma_2),\ \ \sigma_- = \frac{1}{2}(\sigma_1 - i\sigma_2)$$

Dipole moment $\quad \vec{d} = \langle g|\vec{D}|e\rangle, \qquad \text{assuming}\ \ \langle g|\vec{D}|g\rangle = \langle e|\vec{D}|e\rangle = 0$

2. Lindblad equation in interaction picture

$$H_I = -\vec{D}\cdot\vec{E}_B$$

$$\frac{d}{dt}\rho(t) = \hat{\gamma}_0(1+N(\omega_0))\left(\sigma_-\rho(t)\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-,\rho(t)\}\right) + \hat{\gamma}_0 N(\omega_0)\left(\sigma_+\rho(t)\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+,\rho(t)\}\right) = \mathcal{L}_0[\rho]$$

$\mathcal{L}_0$: dissipator (super-operator)

where

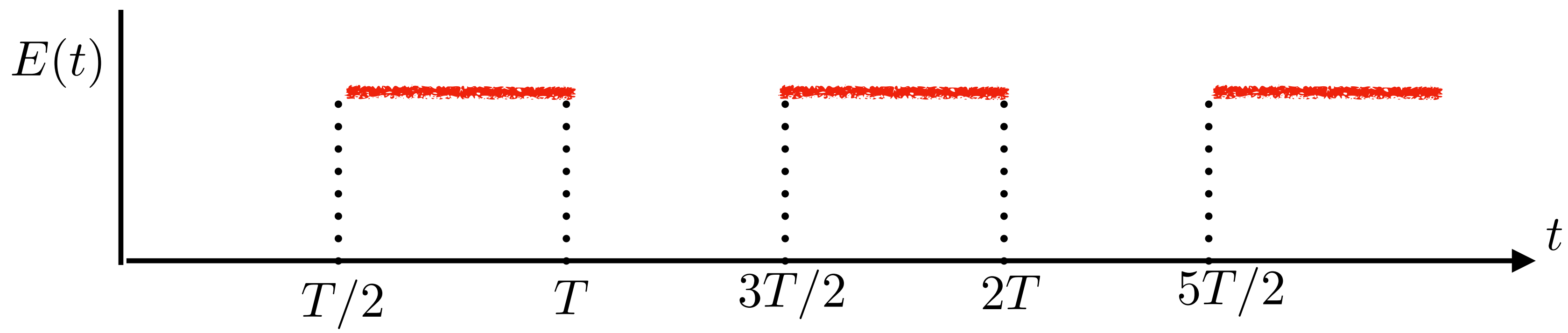
$$\hat{\gamma}_0 = \frac{4\omega_0^2}{3\hbar c}|\vec{d}|^2\ ,\quad N(\omega_0) = \frac{1}{e^{\beta\hbar\omega_0}-1}$$

$$\gamma_0 = \hat{\gamma}_0(1+2N(\omega_0)) = \hat{\gamma}_0\coth(\beta\hbar\omega_0/2) \qquad \text{transition rate,}\ \ \text{dissipation rate}$$

Formal solution $\quad \rho(t) = e^{\int_0^t d\tau\mathcal{L}_0}\rho(0) \quad \longrightarrow \rho_{eq} = \frac{e^{-\beta H_0}}{Z_0}\ \ \text{as}\ t\to\infty$

II. A simple Floquet system

1. A simple Floquet system by tuning a constant electric field piecewise and periodic in time



For $\quad (2n-1)T/2 < t < nT$

$$
\begin{aligned}
H_1 &= H_0 - \vec{D}\cdot\vec{E} \\
&= \frac{\hbar\omega_0}{2}\sigma_3 - (|e\rangle\langle e| + |g\rangle\langle g|)\vec{D}(|e\rangle\langle e| + |g\rangle\langle g|)\cdot\vec{E} \\
&= \frac{\hbar\omega_0}{2}\sigma_3 - \vec{d}\cdot\vec{E}\ (|e\rangle\langle g| + |g\rangle\langle e|) \\
&= \frac{\hbar\omega_0}{2}\begin{pmatrix} 1 & c \\ c & -1 \end{pmatrix} \qquad \text{where} \quad c = -\vec{d}\cdot\vec{E}/(\hbar\omega_0/2)
\end{aligned}
$$

II. A simple Floquet system

2. H_1-basis

$$H_1 = \frac{\hbar\omega_0\sqrt{\alpha}}{2}\ \sigma_3' = \frac{\hbar\omega_1}{2}\ \sigma_3' \qquad \text{where } \alpha = 1 + c^2$$

$$\sigma_3' = |e'\rangle\langle e'| - |g'\rangle\langle g'|$$

$$|e'\rangle = \frac{c}{2\sqrt{\alpha(\sqrt{\alpha}-1)}}\begin{pmatrix} 1 \\ -(\sqrt{\alpha}-1)/c \end{pmatrix}$$

$$|g'\rangle = \frac{c}{2\sqrt{\alpha(\sqrt{\alpha}+1)}}\begin{pmatrix} 1 \\ (\sqrt{\alpha}+1)/c \end{pmatrix}$$

Transfer matrix

$$U = \begin{pmatrix} \langle e'|e\rangle & \langle e'|g\rangle \\ \langle g'|e\rangle & \langle g'|g\rangle \end{pmatrix}$$

$$= \frac{c}{\sqrt{2\alpha}}\begin{pmatrix} \frac{1}{\sqrt{\sqrt{\alpha}-1}} & -\frac{\sqrt{\sqrt{\alpha}-1}}{c} \\ \frac{1}{\sqrt{\sqrt{\alpha}+1}} & \frac{\sqrt{\sqrt{\alpha}+1}}{c} \end{pmatrix}$$

II. A simple Floquet system

3. Lindblad equation in H_1 -basis

$$\frac{d}{dt}\rho = \hat{\gamma}_0'(1+N(\omega_1))\left(\sigma_-'\rho\sigma_+' - \frac{1}{2}\{\sigma_+'\sigma_-', \rho\}\right) + \hat{\gamma}_0' N(\omega_1)\left(\sigma_+'\rho\sigma_-' - \frac{1}{2}\{\sigma_-'\sigma_+', \rho\}\right)$$

$$\hat{\gamma}_0' = \frac{4\omega_1^2}{3\hbar c}|\vec{d}_1|^2 = \frac{4\omega_0^2\alpha}{3\hbar c}\underbrace{|\langle e'|U^{\mathrm{t}}\vec{D}U|g'\rangle|^2}_{=|\vec{d}|^2/\alpha} = \hat{\gamma}_0$$

$$N(\omega_1) = \frac{1}{e^{\beta\hbar\omega_0\sqrt{\alpha}} - 1}$$

$$\gamma_1 = \hat{\gamma}_0(1+2N(\omega_1)) = \gamma_0 \coth(\hbar\omega_0\sqrt{\alpha}/2)$$

a new dissipation rate for an external electric field

III. Time evolution

1. Time evolution for an infinitesimal time

For a 2×2 hermitian matrix A

$$e^{\mathcal{L}dt}A \simeq (1 + dt\mathcal{L})A$$

$$= A + dt\left[\underbrace{\hat{\gamma}_0 N}_{\tilde{\gamma}}(A_{11} + A_{22})\sigma_3 - \underbrace{\hat{\gamma}_0(2N+1)}_{\gamma}\left(A_{11}\sigma_3 + \frac{1}{2}A_{12}\sigma_+ + \frac{1}{2}A_{12}^*\sigma_-\right)\right]$$

$$= \begin{pmatrix} (1-\gamma dt)A_{11} + \tilde{\gamma}dt & (1-\gamma dt/2)A_{12} \\ (1-\gamma dt/2)A_{12}^* & (1-\gamma dt)A_{22} + (\gamma - \tilde{\gamma})(A_{11} + A_{22})dt \end{pmatrix}$$

$$\left[e^{\mathcal{L}dt}\right]^n A = \begin{pmatrix} \tilde{A}_{11} & (1-\gamma dt/2)^n A_{12} \\ (1-\gamma dt/2)^n A_{12}^* & \tilde{A}_{22} \end{pmatrix}$$

$$\tilde{A}_{11} = (1-\gamma dt)^n A_{11} + \tilde{\gamma}dt(A_{11} + A_{22})(1 + (1-\gamma dt) + \cdots + (1-\gamma dt)^{n-1})$$

$$= (1-\gamma dt)^n A_{11} + \tilde{\gamma}(A_{11} + A_{22})dt\frac{1-(1-\gamma dt)^{n-1}}{1-(1-\gamma dt)}$$

$$\tilde{A}_{22} = (1-\gamma dt)^n A_{22} + (\gamma - \tilde{\gamma})(A_{11} + A_{22})dt\frac{1-(1-\gamma dt)^{n-1}}{\gamma dt}$$

III. Time evolution

2. Time evolution for a finite time

$$n \to \infty, \quad ndt \to t$$

$$e^{\int_0^t d\tau \mathcal{L}} A = \begin{pmatrix} e^{-\gamma t} A_{11} + \frac{\tilde{\gamma}}{\gamma}(1 - e^{-\gamma t})(A_{11} + A_{22}) & e^{-\gamma t/2} A_{12} \\ e^{-\gamma t/2} A_{12}^* & e^{-\gamma t} A_{22} + \left(1 - \frac{\tilde{\gamma}}{\gamma}\right)(1 - e^{-\gamma t})(A_{11} + A_{22}) \end{pmatrix}$$

$$\frac{\tilde{\gamma}}{\gamma} = \frac{N(\omega)}{2N(\omega) + 1} = \frac{e^{-\beta\hbar\omega/2}}{e^{\beta\hbar\omega/2} + e^{-\beta\hbar\omega/2}}$$

$$\gamma = \gamma_0 \coth(\beta\hbar\omega/2)$$

3. Periodic Steady state

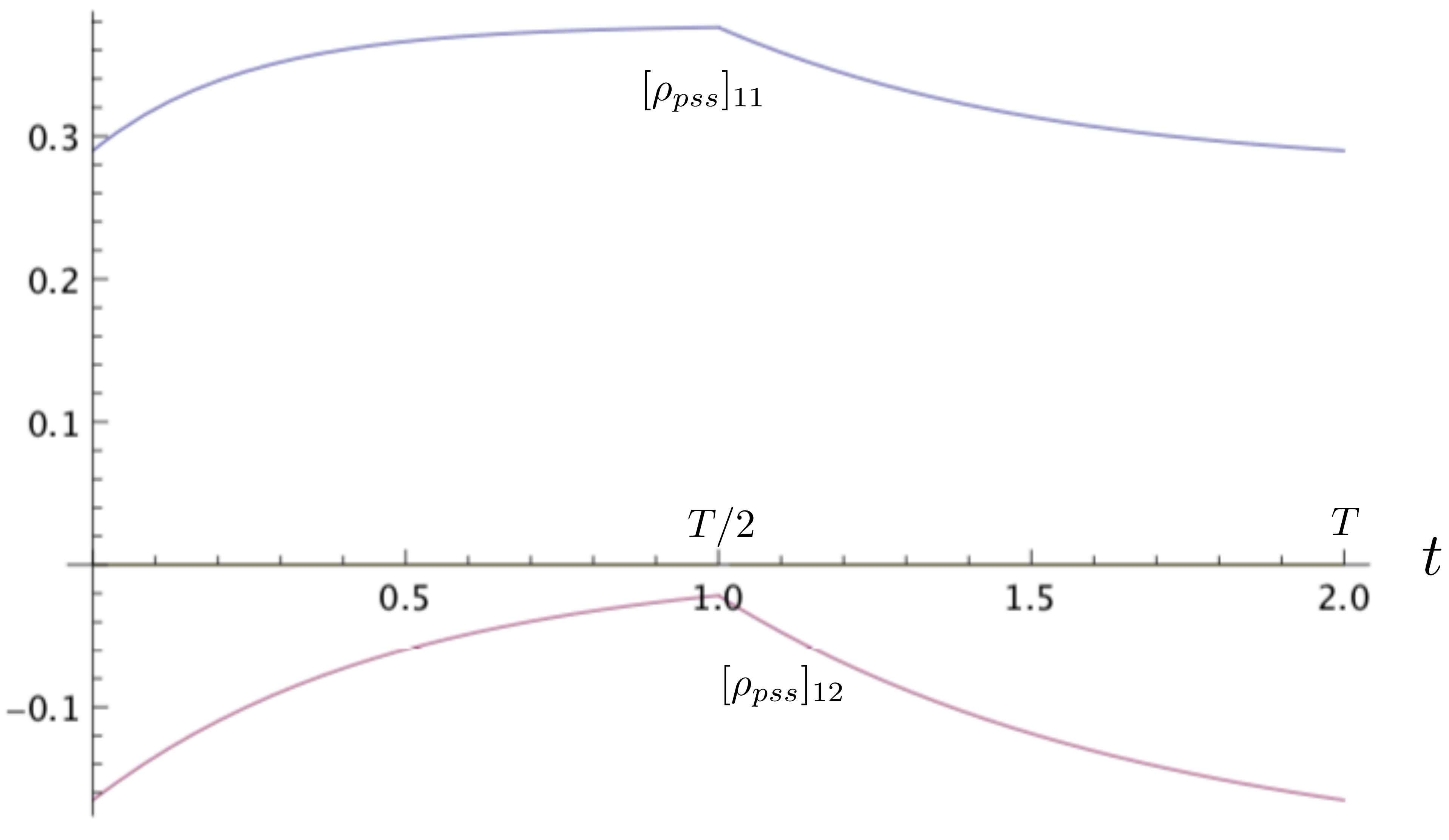
$$A = \rho_{pss}(t) = \rho_{pss}(t + T)$$

$$e^{\int_0^{T/2} d\tau \mathcal{L}_0} \rho_{pss}(0) = \rho_{pss}(T/2)$$

$$e^{\int_T^{T/2} d\tau \mathcal{L}_1} \rho_{pss}(T/2) = \rho_{pss}(0)$$

III. Time evolution

Density matrix for periodic steady state



IV. Fluctuation theorem (within Lindblad)

1. For an isolated system $H = H_S(t) + H_B + H_I$ $\Delta H = W$

· Gallavotti-Cohen symmetry $G(\lambda) = \langle e^{-\lambda\beta H(t)} e^{\lambda\beta H(0)} \rangle$ IC: equilibrium

$$G(\lambda) = G_R(1-\lambda) e^{\beta\Delta F}$$ detailed fluctuation theorem

· Generalized Jarzynski relation

$$\left\langle T \exp\left[\int_0^t d\tau \frac{\partial \rho_{ss}}{\partial \tau} \rho_{ss}^{-1}\right]\right\rangle = 1, \quad \rho_{ss} = e^{\beta F(t)} e^{-\beta H(t)}$$

· Entropy production $S = -\ln \rho_S + \beta H_B$ IC: product state $\rho_B \otimes \rho_S$

$$\langle e^{-S(t)} e^{S(0)} \rangle = 1$$ integral fluctuation theorem

Proof of generalized Jarzynski relation

$$\mathcal{U}(t, t-dt) = e^{dt\mathcal{L}(t-dt)}$$

Note: $\mathcal{L}(t-dt)\rho_{ss}(t-dt, \underbrace{\alpha_{t-dt}}_{\text{protocol}}) = 0$ or $\mathcal{U}(t, t-dt)\rho_{ss}(t-dt, \alpha_{t-dt}) = \rho_{ss}(t, \alpha_{t-dt})$

where $\rho_{ss}(t, \alpha_t) = e^{\beta F(\alpha_t)} e^{-\beta H(\alpha_t)}$

$$\begin{aligned} 1 = \mathrm{Tr} \cdots &\left[\rho_{ss}^{-1}(t, \alpha_{t-dt}) \mathcal{U}(t, t-dt) \rho_{ss}(t-dt, \alpha_{t-dt})\right] \\ \cdots &\left[\rho_{ss}^{-1}(2dt, \alpha_{dt}) \mathcal{U}(2dt, dt) \rho_{ss}(dt, \alpha_{dt})\right] \\ \cdot &\left[\rho_{ss}^{-1}(dt, \alpha_0) \mathcal{U}(dt, 0) \rho_{ss}(0, \alpha_0)\right] \end{aligned}$$

IV. Fluctuation theorem (within Lindblad)

Rearranging

$$1 = \mathrm{Tr} \cdots \underbrace{\left[\rho_{ss}(t,\alpha_t)\rho_{ss}^{-1}(t,\alpha_{t-dt})\right]}\mathcal{U}(t,t-dt)\cdots\mathcal{U}(2dt,dt)\left[\rho_{ss}(dt,\alpha_{dt})\rho_{ss}^{-1}(dt,\alpha_0)\right]\mathcal{U}(dt,0)\rho_{ss}(0,\alpha_0)$$

$$\rho_{ss}(t,\alpha_t)\rho_{ss}^{-1}(t,\alpha_{t-dt}) = \left[\rho_{ss}(t,\alpha_{t-dt}) + \dot{\alpha}_t \frac{\partial}{\partial \alpha_t}\rho_{ss}(t,\alpha_{t-dt})\right]\rho_{ss}^{-1}(t,\alpha_{t-dt})$$

$$= 1 + dt\frac{\partial}{\partial t}\rho_{ss}(t,\alpha_{t-dt})\cdot\rho_{ss}^{-1}(t,\alpha_{t-dt})$$

$$\simeq \exp\left[dt\frac{\partial \rho_{ss}}{\partial t}\rho_{ss}^{-1}\right]$$

General Jarzynski equality

$$\text{Therefore} \quad 1 = \left\langle T\exp\left[\int_0^t d\tau \frac{\partial \rho_{ss}}{\partial t}\rho_{ss}^{-1}\right]\right\rangle \quad \neq \left\langle \exp\left[\beta\Delta F - \beta\int_0^t d\tau \dot{H}\right]\right\rangle$$

$$\frac{\partial}{\partial t}e^{\beta(F-H)} \neq \beta(\dot{F} - \partial H/\partial t)e^{\beta(F-H)}$$

IV. Fluctuation theorem (within Lindblad)

2. FT for a Floquet system driven by a piecewise constant protocol within the Lindblad equation

$$\{H_0,\ \mathcal{L}_0\} \to \{H_1,\ \mathcal{L}_1\} \to \{H_0,\ \mathcal{L}_0\} \to \{H_1,\ \mathcal{L}_1\}, \to \cdots$$

$$\mathcal{U}_0(t',t) = e^{\int_t^{t'} d\tau \mathcal{L}_0},\ \ \mathcal{U}_1(t',t) = e^{\int_t^{t'} d\tau \mathcal{L}_1}$$

Work $\quad W = H_1 - H_0 \quad$ at $t = T/2,\ 3T/2,\ 5T/2, \ldots$

$\quad W = H_0 - H_1 \quad$ at $t = T,\ 2T,\ 3T, \ldots$

Generating function for work

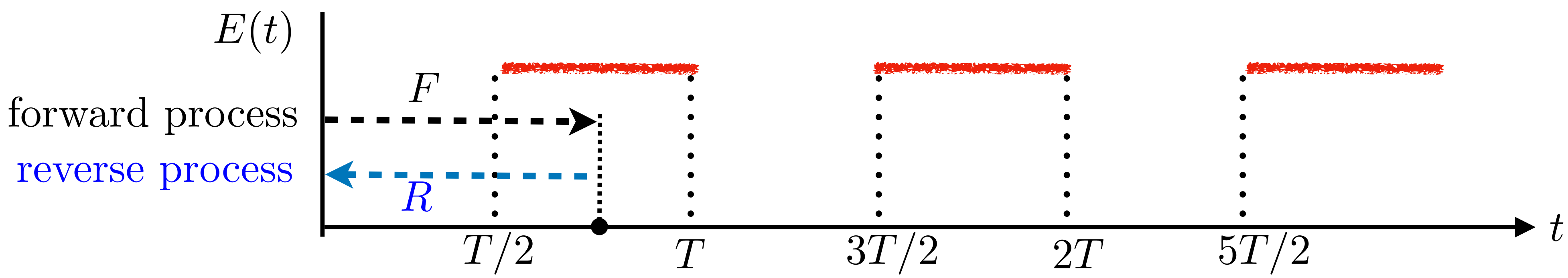
$$G(\lambda) = \mathrm{Tr} \cdots e^{-\lambda\beta H_0} e^{\lambda\beta H_1} \mathcal{U}_1(T, T/2) e^{-\lambda\beta H_1} e^{\lambda\beta H_0} \mathcal{U}_0(T/2, 0) \frac{e^{-\beta H_0}}{Z_0} \qquad \text{cf.} \quad \langle e^{-\lambda\beta W} \rangle$$

Jarzynski equality holds in the original form.

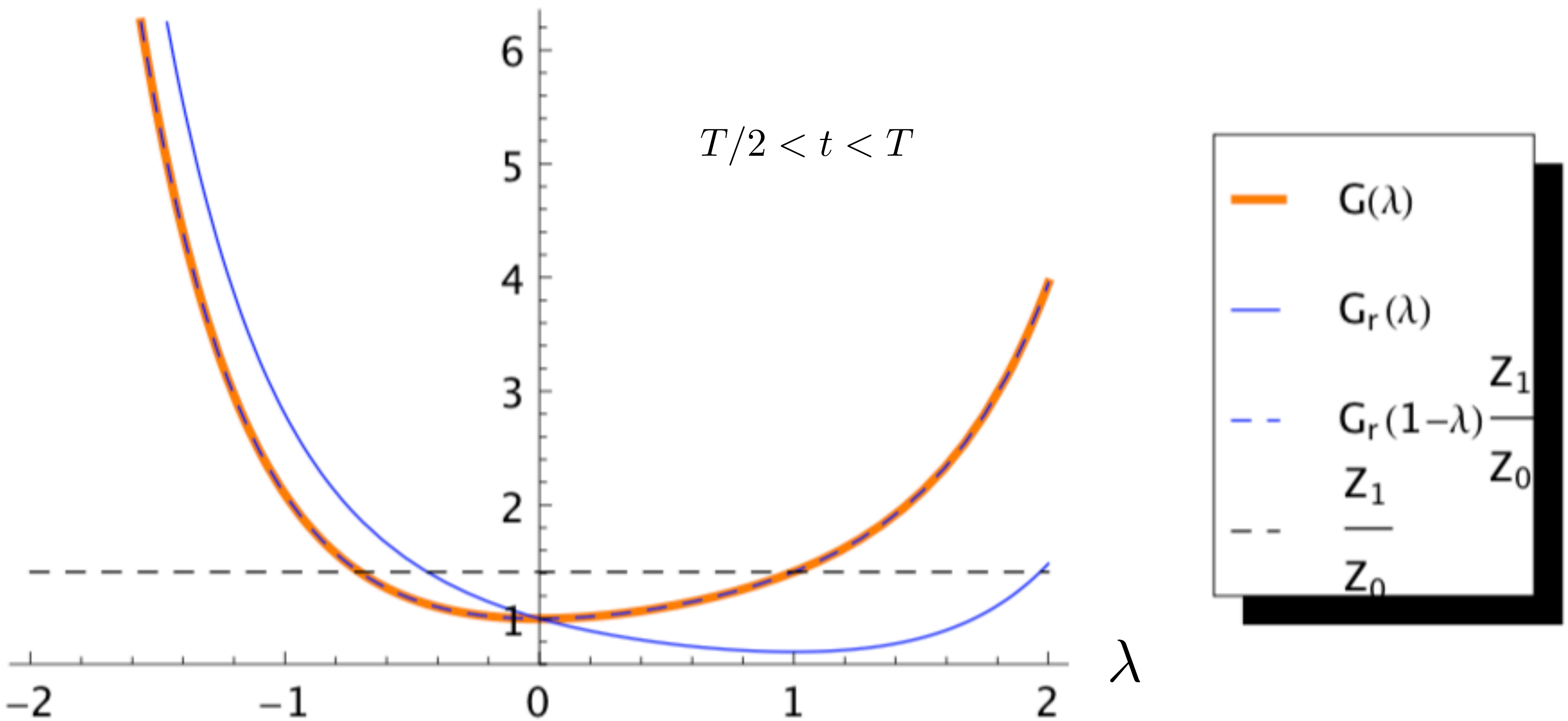
$$G(1) = \mathrm{Tr} \cdots e^{-\beta H_0} e^{\beta H_1} \underbrace{\mathcal{U}_1(T, T/2) e^{-\beta H_1}}_{e^{-\beta H_1}} e^{\beta H_0} \underbrace{\mathcal{U}_0(T/2, 0) \frac{e^{-\beta H_0}}{Z_0}}_{e^{-\beta H_0}/Z_0}$$

$$= \frac{Z_1}{Z_0} = e^{\beta(F_1 - F_0)} \quad \text{or} \quad 1$$

IV. Fluctuation theorem (within Lindblad)



$\beta\hbar\omega_0/2 = 1,\ c = -\vec{E}\cdot\vec{d}/(\hbar\omega_0/2) = 1$



GC-symmetry holds! $\quad G(\lambda) = G_r(1-\lambda)\dfrac{Z_1}{Z_0}$

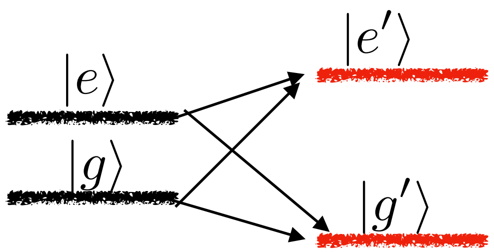
IV. Fluctuation theorem (within Lindblad)

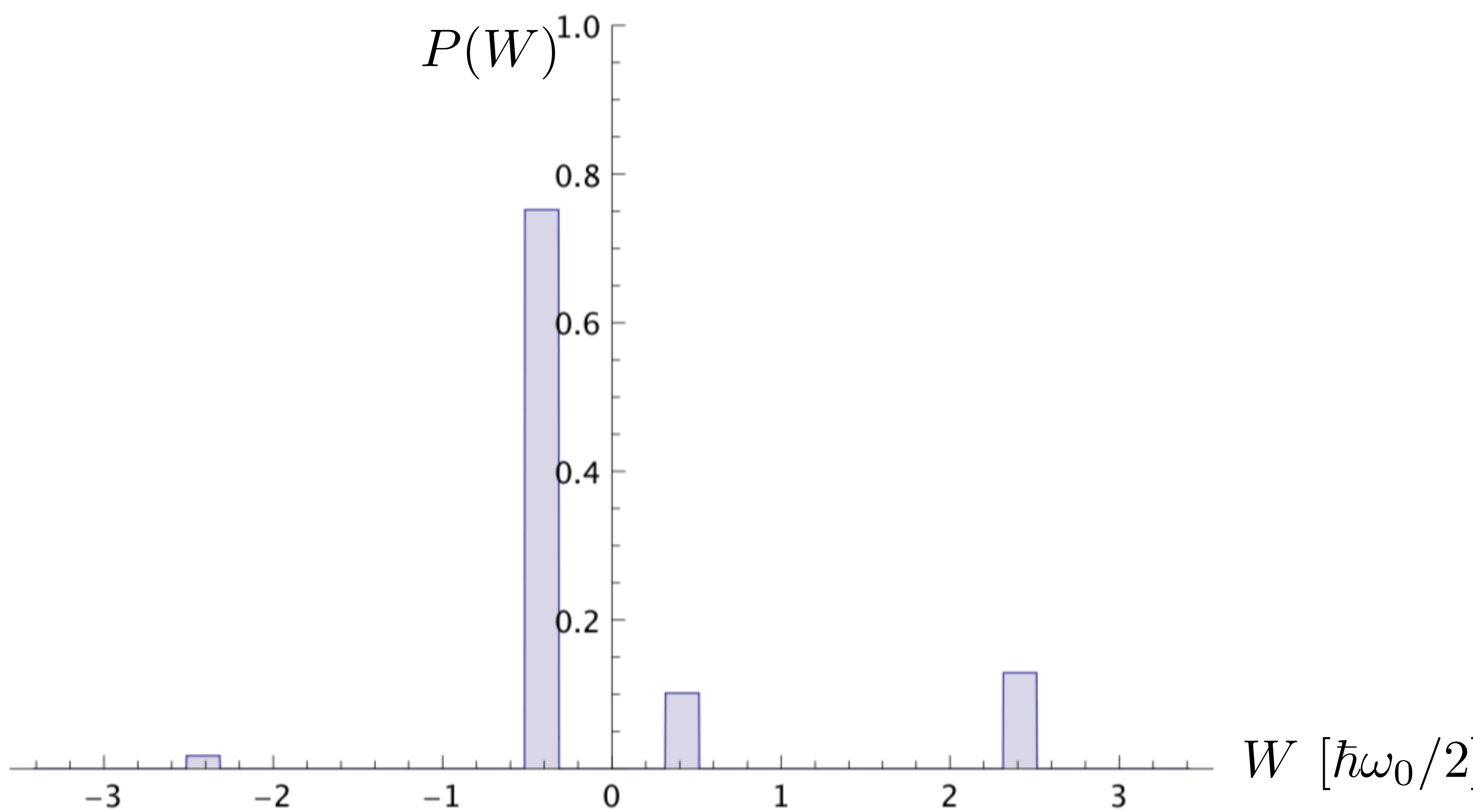
Work distribution

$$P(W) = \int_{-\infty}^{\infty} \frac{d\lambda}{2\pi} e^{i\lambda W} G(i\lambda)$$

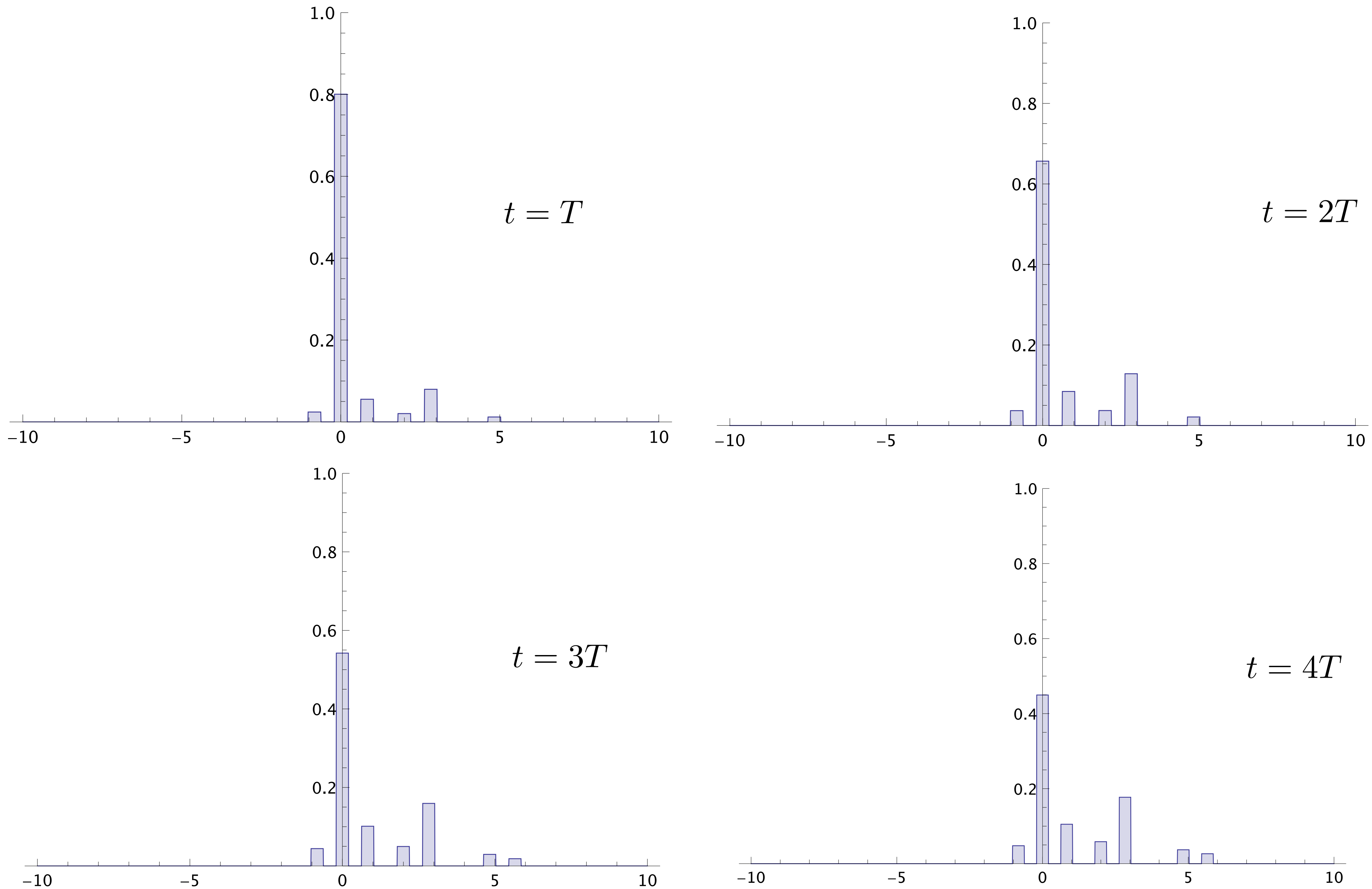
$\beta\hbar\omega_0/2 = 1,\ c = -\vec{E}\cdot\vec{d}/(\hbar\omega_0/2) = 1$

Delta peaks at $W/(\hbar\omega_0/2) = \pm 1 \pm (1+\sqrt{2})$ for $T/2 < t < T$





More delta peaks as t increases.



Many peaks with small weights are not shown.
It is hard to find rigorous P(W) at large t.

V. Summary

1. **A nonequilibrium for a simple Floquet system is studied by using the Lindblad equation.**

2. **GC-symmetry is shown to hold rigorously.**

3. **The generating function for work is obtained and can be used to find work distribution function. Similarly, heat distribution can be found.**

4. **Not shown in the talk, it is observed for our specific case**

$$\langle -\Delta \ln \rho + \beta Q \rangle > 0 \qquad \langle Q \rangle = \mathrm{Tr} H(t) \mathcal{L} \rho$$

   but the corresponding FT is not found.

5. **The strong coupling theory for general time-protocol will be investigated.**