Canonical Quantization of Brownian Motion and Quantum Thermodynamics

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(collaboration with Fernando Nicacio (IF UFRJ))

Phys. Lett. A494, 129277 (2024).

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Thermodynamics

1. Systems involve macroscopic degrees of freedom (thermodynamical limit, small fluctuation)

2. Initial and final states of processes are in equilibrium.

Thermodynamics

1. Systems involve macroscopic degrees of freedom (thermodynamical limit, small fluctuation)

→ Small systems

2. Initial and final states of processes are in equilibrium. → Time evolutions from arbitrary states

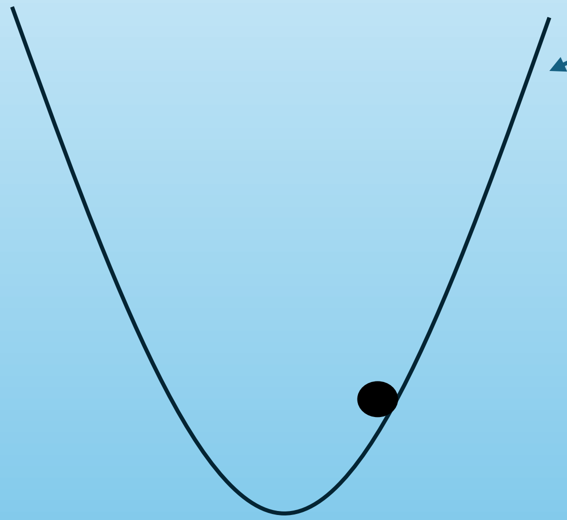
Attempts to this generalization:

- classical side → Stochastic thermodynamics
- quantal side → Quantum thermodynamics

These formulations are yet under construction.

Stochastic Thermodynamics

Stochastic thermodynamics (stochastic energetics)

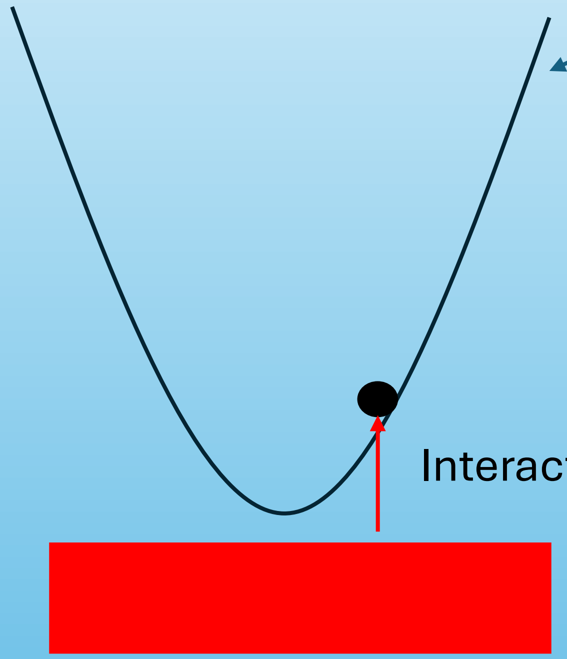


External confinement potential $V(x, \lambda_t)$

$$dx_t = \frac{p_t}{m} dt$$

$$dp_t = -\partial V(q_t, \lambda_t) dt$$

Stochastic thermodynamics (stochastic energetics)



Standard Brownian motion

$$dx_t = \frac{p_t}{m} dt$$

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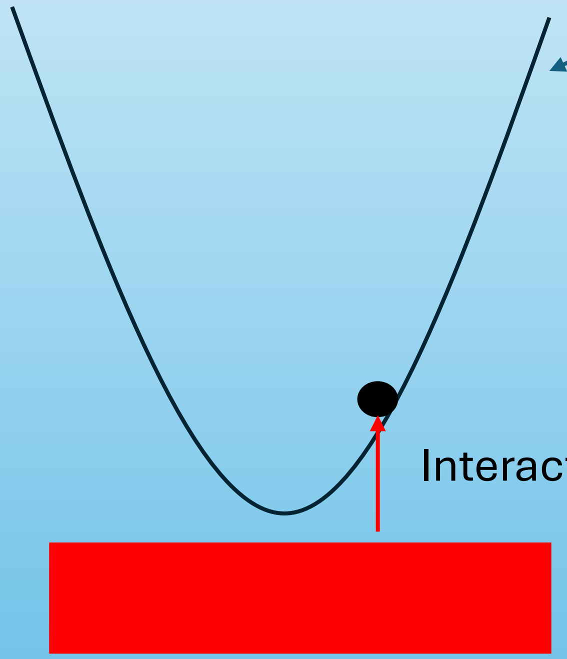
Stochastic thermodynamics (stochastic energetics)

External confinement potential $V(x,\lambda_t)$

Standard Wiener process (Gaussian white noise)



Interaction with heat bath

Heat bath of β^{-1}

1. dissipation
2. fluctuation

Standard Brownian motion

$$dx_t = \frac{p_t}{m}dt$$

$$dp_t = -\partial V(q_t,\lambda_t)dt - \gamma\frac{p_t}{m}dt + \sqrt{\frac{2\gamma}{\beta}}dB_t$$

Stochastic thermodynamics (stochastic energetics)

Sekimoto, “Stochastic Energetics” (Springer, 2010)

Heat absorbed by the system is interpreted as a **work** done by the heat bath on the system.

$$dQ_t^c = \int \mathrm{d}\Gamma_0 \mathrm{f}_0\left(\Gamma_0\right) \mathrm{E}\left[\left(-\gamma \frac{p_t}{m} dt + \sqrt{\frac{2\gamma}{\beta}}\right) \circ dx_t\right]$$

$\mathrm{E}[\cdots]$: ensemble average for thermal fluctuation (Wiener)

$d\Gamma_0 = dq_0 dp_0$

$f_0(\Gamma_0)$: initial phase space distribution

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$\mathrm{E}[\cdots]$: ensemble average for thermal fluctuation (Wiener)

Energy

$$U_t^c = \int d\Gamma_0 f_0(\Gamma_0) \mathrm{E}\left[\frac{p_t^2}{2m} + V(x_t, \lambda_t)\right]$$

Work by heat bath

$$dW_t^c = \int d\Gamma_0 f_0(\Gamma_0) \mathrm{E}\left[d\tilde{W}_t^c\right] \qquad d\tilde{W}_t^c := \frac{\partial V(q_t, \lambda_t)}{\partial \lambda_t} d\lambda_t$$

$$d\Gamma_0 = dq_0 dp_0$$

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$\mathrm{E}[\cdots]$: ensemble average for thermal fluctuation (Wiener)

First law

$$U_{t_f}^c - U_{t_i}^c = dQ_t^c + dW_t^c$$

Energy

$$U_t^c = \int d\Gamma_0 f_0(\Gamma_0) \mathrm{E}\left[\frac{p_t^2}{2m} + V(x_t, \lambda_t) \right]$$

Work by heat bath

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Information entropy

$$S_c = -k_B \int d\Gamma\, f(\Gamma, t) \ln f(\Gamma, t)$$

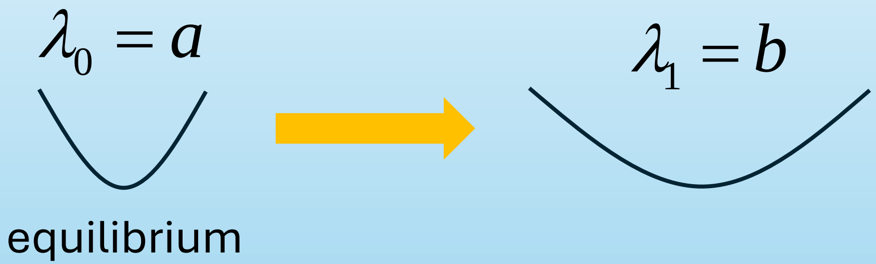
Phase space distribution

Second law

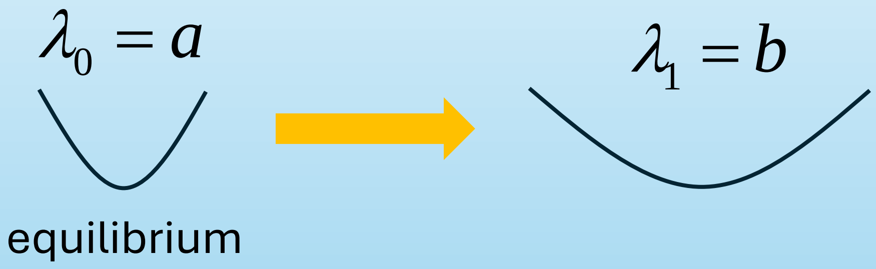
$$\frac{dS_c}{dt} - k_B \beta \frac{dQ_t^c}{dt} \geq 0$$

The equality is satisfied for the equilibrium distribution, $f_{eq} = \frac{1}{Z} e^{-\beta\left(\frac{p^2}{2m} + V(x, \lambda_\infty)\right)}$

Jarzynski equality



Jarzynski equality

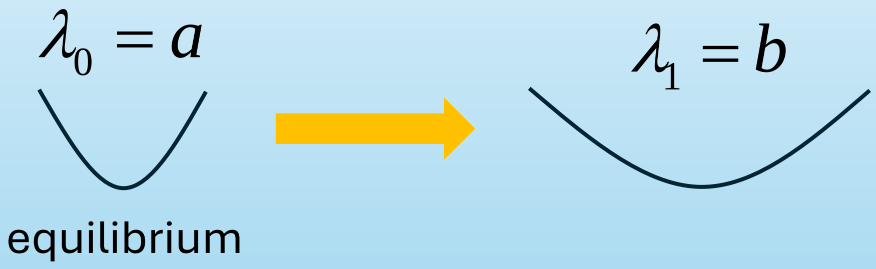


Let us consider the external perturbation characterized by $\lambda_0 = a \longrightarrow \lambda_1 = b$. Then the averaged work in this process is

$$W_{0\to 1}^{c} = \int d\Gamma_0 f_{eq}\left(\Gamma_0\right) \mathrm{E}\left[\int_0^1 d\tilde{W}_t^{c}\right]$$

Then, for the above process, we can show

Jarzynski equality



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$$W^c_{0\to 1} = \int d\Gamma_0 f_{eq}(\Gamma_0) \mathrm{E}\left[\int_0^1 d\tilde{W}^c_t\right]$$

Then, for the above process, we can show

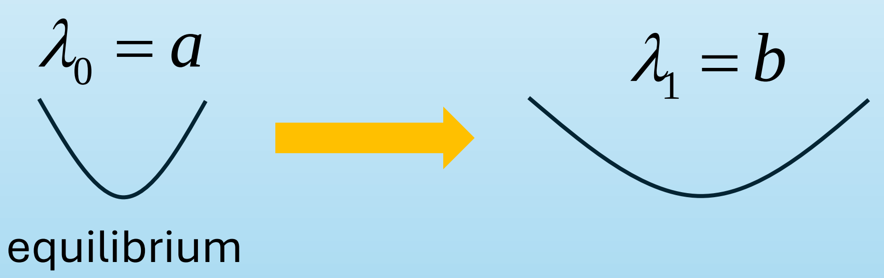
Jarzynski equality

$$\int d\Gamma_0 f_{eq}(\Gamma_0) \mathrm{E}\left[\exp\left(-\beta\left(\int_0^1 d\tilde{W}^c_t - \Delta F\right)\right)\right] = 1$$

$$\Delta F = \beta^{-1}(-\ln Z_1 + \ln Z_0) \qquad Z_t = \int d\Gamma e^{-\beta\left(\frac{p^2}{2m} + V(x,\lambda_t)\right)}$$

Jarzynski equality is one of fluctuation theorems.

Jarzynski equality



Let us consider the external perturbation characterized by $\lambda_0 = a \longrightarrow \lambda_1 = b$. Then the averaged work in this process is

$$W^c_{0\to1} = \int d\Gamma_0 f_{eq}(\Gamma_0) \mathrm{E}\left[\int_0^1 d\tilde{W}^c_t\right]$$

Then, for the above process, we can show

Jarzynski equality

$$\int d\Gamma_0 f_{eq}(\Gamma_0) \mathrm{E}\left[\exp\left(-\beta\left(\int_0^1 d\tilde{W}^c_t - \Delta F\right)\right)\right] = 1$$

second law

$$-W^c_{0\to1} \leq -\Delta F$$

$$\Delta F = \beta^{-1}(-\ln Z_1 + \ln Z_0) \qquad Z_t = \int d\Gamma e^{-\beta\left(\frac{p^2}{2m} + V(x,\lambda_t)\right)}$$

There always exist stochastic events which change in an opposite direction to the mean behavior of entropy.

Jarzynski equality is one of fluctuation theorems.

Of course, stochastic thermodynamics is not applicable to extremely small systems where quantum fluctuation should be considered.

How do we introduce a quantum dissipative model which is thermodynamically consistent?

Quantum Thermodynamics

CPTP map

What is the requirements for the density matrix in open quantum systems (system + environment)?

Dynamical map (time evolution)

$$\hat{\rho} \rightarrow M\left[\hat{\rho}\right]$$

1. Linear time evolution

$$M\left[a\hat{\rho}_1 + b\hat{\rho}_2\right] = aM\left[\hat{\rho}_1\right] + bM\left[\hat{\rho}_2\right]$$

2. Completely positive

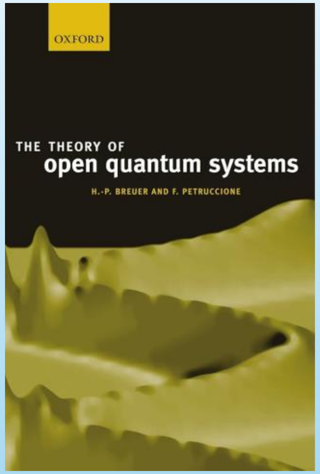
$$\hat{\rho}_{AB} \geq 0 \longrightarrow M_A \otimes I_B\left[\hat{\rho}_{AB}\right] \geq 0$$

3. Trace conservation

$$\mathrm{Tr}\left[\hat{\rho}\right] = \mathrm{Tr}\left[M\left[\hat{\rho}\right]\right]$$

The time evolutions satisfying these conditions are called completely positive and trace-preserving (CPTP) maps.
We require that open quantum dynamics is described by the CPTP evolution.

How do we obtain non-eq. dynamics?

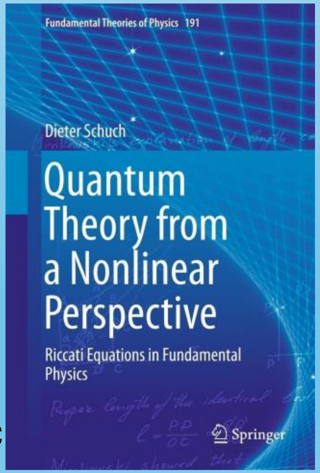


There is no systematic method to obtain non-equilibrium dynamics consistent with the CPTP map for arbitrary Hamiltonian.

Systematic coarse-graining of environment degrees of freedom

1. Projection operator method (Nakajima-Zwanzig, Mori, Kawasaki-Gunton, Shibata-Hashitsume, etc)

2. Coarse-graining based on path integrals (influence functional, closed time path, etc)



Quantization of classical dissipative system

1. Canonical quantization (Caldirola, Kanai, Bateman, etc)

2. Non-linear Schrödinger equation through the Ehrenfest theorem (Kostin, Hasse, Schuch, etc

Non-Hermitian (PT-symmetric) quantum mechanics

GKSL equation

In the standard discussions of quantum thermodynamics, we often employ the equation proposed by Lindblad (1976) and Gorini-Kossakowski-Sudarshan (1976).

irreversible current

$$\frac{d}{dt}\hat{\rho} = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}\right] + D\left[\hat{\rho}\right] \qquad D\left[\hat{\rho}\right] = \sum_i \gamma_i \left\{ -\frac{1}{2}\left[\hat{L}_i^\dagger \hat{L}_i, \hat{\rho}\right] + \hat{L}_i \hat{\rho} \hat{L}_i^\dagger \right\}$$

reversible current

$\gamma_i \geq 0$: Dissipative coefficients

$\hat{L}_i$: jump (Lindblad) operator

1. The Gorini-Kossakowski-Sudarshan-Lidblad (GKSL) equation is an example of the CPTP evolution.
2. There is no systematic method to define the Lindblad operator.
3. It is not clear whether this is applicable to describe thermal relaxation processes.

Application to harmonic oscillator

For the harmonic oscillator Hamiltonian, we can find the Lindblad operator which is consistent with thermodynamics

$$H = \hbar\omega\left(\hat{a}^{\dagger}\hat{a} + \frac{1}{2}\right)$$

$$\hat{L}_{+} = \hat{a} = \hat{L}_{-}^{\dagger}$$

$$\hat{L}_{-} = \hat{a}^{\dagger} = \hat{L}_{+}^{\dagger}$$

$$\frac{\gamma_{-}}{\gamma_{+}} = e^{-\beta\hbar\omega}$$

Detailed balance condition

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$$\hat{L}_- = \hat{a}^\dagger = \hat{L}_+^\dagger$$

$$\frac{\gamma_-}{\gamma_+} = e^{-\beta\hbar\omega}$$

Detailed balance condition

Even if this is not satisfied, the equation is CPTP, but does not describe thermal equilibration.

Quantum heat $dQ_t^q := \mathrm{Tr}\left[\hat{H} d\hat{\rho}_t\right]$

von Neumann entropy $S_t^q := -k_B \mathrm{Tr}\left[\hat{\rho}_t \ln \hat{\rho}_t\right]$

$$\frac{dS_t^q}{dt} - k_B \beta^{-1} \frac{dQ_t^q}{dt} \geq 0$$

The GKSL equation is consistent with thermodynamics at least in the application to the harmonic oscillator.

We want to find a systematic procedure to obtain open quantum dynamics which is consistent with CPTP and describe thermal relaxation processes.

Our strategy is……

Brownian motion → Stochastic thermodynamics

CPTP evolution → Quantum thermodynamics

Our strategy is……

More general theory of Brownian motion (but in flat spacetime)

1) propose

Brownian motion → Stochastic thermodynamics

CPTP evolution → Quantum thermodynamics

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More general theory of Brownian motion (but in flat spacetime)

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3) Canonical quantization

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Generalized Brownian Motion

Generalized Brownian motion

Koide&Nicacio, Phys. Lett. A494, 129277 (2024).

Let us consider a thermal relaxation process with a general Hamiltonian H.

Our new model of Brownian motion for the i-th particle

$$d\vec{q}_{(i)t} = \frac{\partial H}{\partial \vec{p}_{(i)t}} dt$$

$$d\vec{p}_{(i)t} = -\frac{\partial H}{\partial \vec{q}_{(i)t}} dt$$

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$$d\vec{q}_{(i)t} = \frac{\partial H}{\partial \vec{p}_{(i)t}} dt$$

$$d\vec{p}_{(i)t} = -\frac{\partial H}{\partial \vec{q}_{(i)t}} dt - \gamma_{q_i} \frac{\partial H}{\partial \vec{p}_{(i)t}} dt + \sqrt{\frac{2\gamma_{p_i}}{\beta_i}} d\vec{B}_{p(i)t}$$

$$\mathrm{E}\left[dB^{\alpha}_{q(i)t} \right] = \mathrm{E}\left[dB^{\alpha}_{p(i)t} \right] = 0$$

$$\mathrm{E}\left[dB^{\alpha}_{q(i)t} dB^{\beta}_{q(j)t'} \right] = \mathrm{E}\left[dB^{\alpha}_{p(i)t} dB^{\beta}_{p(j)t'} \right] = dt\,\delta_{ij}\delta_{\alpha\beta}\delta_{tt'}$$

$$\mathrm{E}\left[dB^{\alpha}_{q(i)t} dB^{\beta}_{p(j)t'} \right] = 0$$

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$$\mathrm{E}\left[dB^{\alpha}_{q(i)t} dB^{\beta}_{p(j)t'} \right] = 0$$

Thermodynamical quantities

Koide&Nicacio, Phys. Lett. A494, 129277 (2024).

Energy
$$U_t^c = \int d\Gamma_0 f_0(\Gamma_0) \mathrm{E}\left[H(\Gamma_t, \lambda_t) \right]$$

Work
$$dW_t^c = \int d\Gamma_0 f_0(\Gamma_0) \mathrm{E}\left[d\tilde{W}_t^c \right] \qquad d\tilde{W}_t^c := \frac{\partial H(\Gamma_t, \lambda_t)}{\partial \lambda_t} d\lambda_t$$

Heat
$$dQ_{(i)t}^c = \int d\Gamma_0 f_0(\Gamma_0) \sum_\alpha \mathrm{E}\left[\left(-\gamma_{p_i} \frac{\partial H}{\partial p_{(i)t}^\alpha} dt + \sqrt{\frac{2\gamma_{p_i}}{\beta_i}} dB_{p(i)t}^\alpha \right) \circ dq_{(i)t}^\alpha \right]$$
$$- \int d\Gamma_0 f_0(\Gamma_0) \sum_\alpha \mathrm{E}\left[\left(-\gamma_{q_i} \frac{\partial H}{\partial q_{(i)t}^\alpha} dt + \sqrt{\frac{2\gamma_{q_i}}{\beta_i}} dB_{q(i)t}^\alpha \right) \circ dp_{(i)t}^\alpha \right]$$

1. These are reduced to standard quantities by using $H = \frac{p^2}{2m} + V$ and $\gamma_{q_i} = 0$.
2. We can choose even interacting and relativistic Hamiltonians.

Phys. Rev. E83,061111 (2011), J. Phys. Commun. 2, 021001 (2018)

Stochastic energetics

Koide&Nicacio, Phys. Lett. A494, 129277 (2024).

First law

$$U^{c}_{t+dt} - U^{c}_{t} = \sum_{i} dQ^{c}_{(i)t} + dW^{c}_{t}$$

Second law

$$\frac{dS^{c}_{t}}{dt} - \sum_{i=1}^{N} k_B \beta_i^{-1} \frac{dQ^{c}_{(i)t}}{dt} \geq 0 \qquad S^{c}_{t} = -k_B \int d\Gamma f(\Gamma, t) \ln f(\Gamma, t)$$

We can still apply thermodynamical interpretations to this generalized BM.

Canonical quantization and new quantum master equation

Our strategy is……

Most general theory of Brownian motion (but in flat spacetime)

1) propose

2) Thermodynamically consistent

3) Canonical quantization

Brownian motion → Stochastic thermodynamics

GKSL equation → Quantum thermodynamics

Apply quantization to phase space distribution.

Generalized Kramers equation

Koide&Nicacio, Phys. Lett. A494, 129277 (2024).

The phase space distribution

$$f\left(\Gamma,t\right) := \int d\Gamma_0 f_0\left(\Gamma_0\right) \prod_{\alpha,i} \mathrm{E}\left[\delta(q^{\alpha}_{(i)} - q^{\alpha}_{(i)t})\delta(p^{\alpha}_{(i)} - p^{\alpha}_{(i)t})\right]$$

α : Components of vectors

The differential equation of the phase space distribution (generalized Kramers equation) is

$$\partial_t f = -\{f, H\}_{PB} + \sum_{i=1}^{N}\sum_{\alpha=1}^{D} \frac{\gamma_{p_i}}{\beta_i} \left\{ e^{-\beta_i H} \left\{ e^{\beta_i H} f, q^{\alpha}_{(i)} \right\}_{PB}, q^{\alpha}_{(i)} \right\}_{PB} + \sum_{i=1}^{N}\sum_{\alpha=1}^{D} \frac{\gamma_{q_i}}{\beta_i} \left\{ e^{-\beta_i H} \left\{ e^{\beta_i H} f, p^{\alpha}_{(i)} \right\}_{PB}, p^{\alpha}_{(i)} \right\}_{PB}$$

$$\{g,h\}_{PB} = \sum_{i=1}^{N}\sum_{\alpha=1}^{D} \left(\frac{\partial g}{\partial q^{\alpha}_i}\frac{\partial h}{\partial p^{\alpha}_i} - \frac{\partial g}{\partial p^{\alpha}_i}\frac{\partial h}{\partial q^{\alpha}_i} \right)$$

Canonical quantization

Koide&Nicacio, Phys. Lett. A494, 129277 (2024).

$$\{g,h\}_{PB}$$

$$f\left(\Gamma,t\right)$$

$$e^{\pm\beta_i H} f\left(\Gamma,t\right)$$

→

$$-\frac{i}{\hbar}\left[\hat{g},\hat{h}\right] \quad -\frac{i}{\hbar}[\hat{q},\hat{p}]=1$$

$$\hat{\rho}(t)$$

$$e^{\pm\beta_i\hat{H}/2}\hat{\rho}\left(t\right)e^{\mp\beta_i\hat{H}/2}$$

New quantum master equation

Koide&Nicacio, Phys. Lett. A494, 129277 (2024).

$$\frac{d\hat{\rho}}{dt} = \frac{i}{\hbar}\left[\hat{\rho}, \hat{H}\right] + D[\hat{\rho}]$$

$$D[\hat{\rho}] = -\sum_{i=1}^{N}\sum_{\alpha=1}^{D}\frac{\gamma_{p_i}}{\beta_i\hbar^2}\left[e^{-\beta_i\hat{H}/2}\left[e^{\beta_i\hat{H}/2}\hat{\rho}e^{\beta_i\hat{H}/2}, \hat{q}^{\alpha}_{(i)}\right]e^{-\beta_i\hat{H}/2}, \hat{q}^{\alpha}_{(i)}\right]$$
$$-\sum_{i=1}^{N}\sum_{\alpha=1}^{D}\frac{\gamma_{q_i}}{\beta_i\hbar^2}\left[e^{-\beta_i\hat{H}/2}\left[e^{\beta_i\hat{H}/2}\hat{\rho}e^{\beta_i\hat{H}/2}, \hat{p}^{\alpha}_{(i)}\right]e^{-\beta_i\hat{H}/2}, \hat{p}^{\alpha}_{(i)}\right]$$

When all particles interacts with the same beat bath ($\beta_1 = \beta_2 = \cdots = \beta_N = \beta$),
the stationary solution is given by thermal equilibrium state,

$$\frac{d\hat{\rho}_{eq}}{dt} = 0 \qquad \hat{\rho}_{eq} = \frac{1}{Z}e^{-\beta\hat{H}}$$

Is this time evolution CPTP?

Koide&Nicacio, Phys. Lett. A494, 129277 (2024).

Let us consider a harmonic oscillator, $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2 \hat{q}^2$

violates CPTP

$$D[\hat{\rho}] \rightarrow -\frac{1}{2\hbar}\sum_{\mu\nu=1}^{4} \eta_{\mu\nu} \left\{ \left[\hat{L}_\mu^\dagger \hat{L}_\nu , \hat{\rho} \right]_+ - 2\hat{L}_\mu \hat{\rho} \hat{L}_\nu^\dagger \right\} \quad \eta_{\mu\nu} = \mathrm{Diag}(1,1,1,-1)$$

$$\hat{L}_1 = \Gamma_1 \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{q} + \frac{i}{m\omega}\hat{p} \right)$$

$$\hat{L}_2 = \Gamma_2 \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{q} - \frac{i}{m\omega}\hat{p} \right)$$

$$\hat{L}_3 = \sqrt{\delta}\hat{q}$$

$$\hat{L}_4 = \frac{\sqrt{\delta}}{m\omega}\hat{p}$$

$$\Gamma_i = \sqrt{\frac{(\delta+2)\gamma_p}{2\beta m\omega} e^{(-1)^{i+1}\beta\hbar\omega/2}}$$

$$\delta = \frac{\gamma_q}{\gamma_p}(m\omega)^2 - 1$$

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$$\hat{L}_1 = \Gamma_1\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{i}{m\omega}\hat{p}\right)$$

$$\hat{L}_2 = \Gamma_2\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} - \frac{i}{m\omega}\hat{p}\right)$$

$$\hat{L}_3 = \sqrt{\delta}\hat{q}$$

$$\hat{L}_4 = \frac{\sqrt{\delta}}{m\omega}\hat{p}$$

$$\Gamma_i = \sqrt{\frac{(\delta+2)\gamma_p}{2\beta m\omega}e^{(-1)^{i+1}\beta\hbar\omega/2}}$$

$$\delta = \frac{\gamma_q}{\gamma_p}(m\omega)^2 - 1$$

For our master equation to be CPTP, we need to set

$$\delta = 0 \rightarrow \gamma_p = \gamma_q(m\omega)^2$$

Reproduction of GKSL equation

Koide&Nicacio, Phys. Lett. A494, 129277 (2024).

Our master equation is finally reduced to the GKSL equation with the detailed balance condition

$$\frac{d\hat{\rho}_t}{dt} = \frac{i}{\hbar}\left[\hat{\rho}_t, \hat{H}\right] - \frac{1}{2\hbar}\sum_{\mu=\pm}\gamma_\mu\left\{\left[L^\dagger_\mu L_\mu, \hat{\rho}_t\right]_+ - 2L_\mu\hat{\rho}_t L^\dagger_\mu\right\}$$

$$\hat{L}_+ = \left(\hat{q} + \frac{i}{m\omega}\hat{p}\right) \qquad \hat{L}_- = \left(\hat{q} - \frac{i}{m\omega}\hat{p}\right) \qquad \gamma_\pm = e^{\pm\beta\hbar\omega/2}\frac{\gamma_p}{2\hbar\beta}$$

$$\Rightarrow \quad \frac{\gamma_-}{\gamma_+} = e^{-\beta\hbar\omega}$$

We can show the laws analogous to the first and second law.

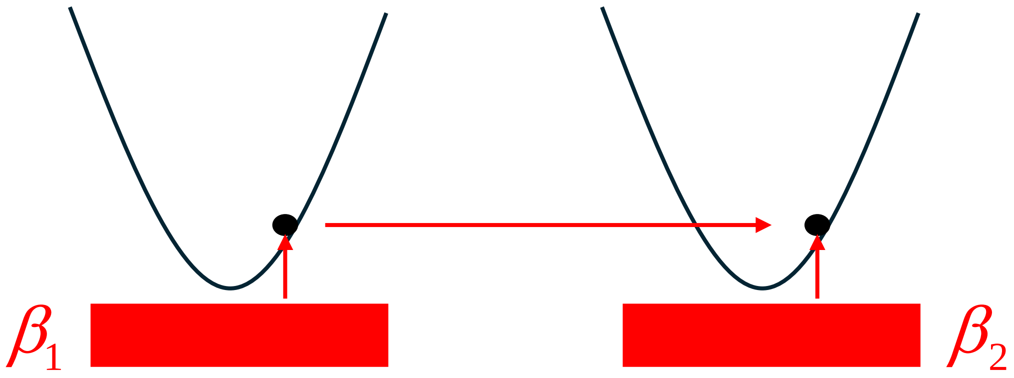
GKSL equation → CPTP, but not always converges toward equilibrium

Our master equation → Not always CPTP, but converges toward equilibrium

CPTP even in other interactions?

Nicacio&Koide in preparation.

Model for heat conduction (network model)



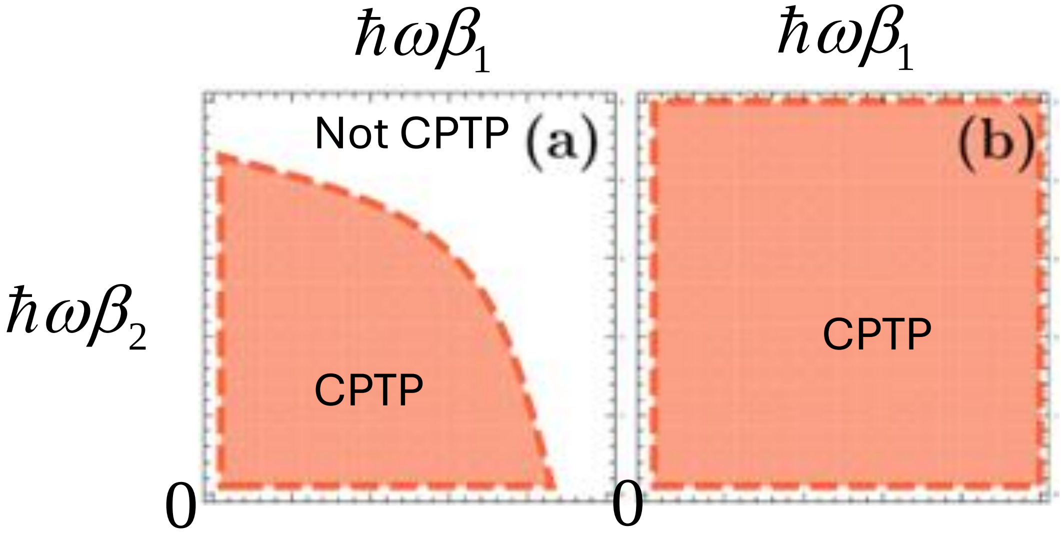
$$\hat{H} = \sum_{i=1}^{2}\left(\frac{\hat{p}_i^2}{2m} + \frac{m}{2}\omega^2\hat{q}_i^2\right) + \frac{K}{2}\left(\hat{q}_1 - \hat{q}_2\right)^2$$

$$m = \omega^{-1}$$

$$K = \omega$$

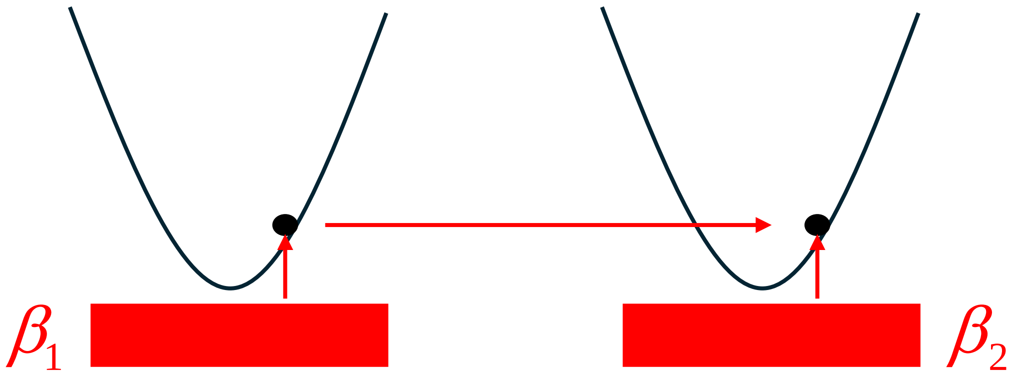
CPTP even in other interactions?

Nicacio&Koide in preparation.



$$\left(\gamma_q, \gamma_p\right) = \quad \left(\frac{1}{4\omega}, \frac{1}{4\omega}\right) \quad \left(\frac{1}{4\omega}, \frac{1}{2\omega}\right)$$

Model for heat conduction (network model)



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$$m = \omega^{-1}$$

$$K = \omega$$

We can find appropriate parameters where our quantum master equation conforms to a CPTP evolution even in the network model.

Other topics

Stochastic energetics in Field theory

Brownian motion for the scalar field

$$d\phi(x_i,t) = (dt)\frac{\delta H}{\delta \Pi(x_i,t)} - (dt)\gamma_\phi \frac{\delta H}{\delta \phi(x_i,t)} + \sqrt{\frac{2\gamma_\phi}{(dx)\beta}} dB^\phi(x_i,t)$$

$$d\Pi(x_i,t) = -(dt)\frac{\delta H}{\delta \phi(x_i,t)} - (dt)\gamma_\Pi \frac{\delta H}{\delta \Pi(x_i,t)} + \sqrt{\frac{2\gamma_\Pi}{(dx)\beta}} dB^\Pi(x_i,t)$$

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Heat

$$dQ_t^{sf} = \int dx\left(-\gamma_\Pi \frac{\delta H}{\delta\Pi} + \sqrt{\frac{2\gamma_\Pi}{dx\beta}}\frac{dB^\Pi}{dt}\right)\circ d\phi - \int dx\left(-\gamma_\phi \frac{\delta H}{\delta\phi} + \sqrt{\frac{2\gamma_\phi}{dx\beta}}\frac{dB^\phi}{dt}\right)\circ d\Pi$$

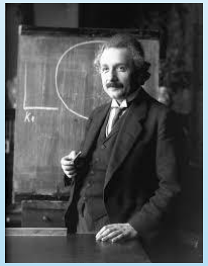
Law analogous to the second law

$$\frac{dS_t^{sf}}{dt} - k_B\beta^{-1}\frac{dQ_t^{sf}}{dt} \geq 0$$

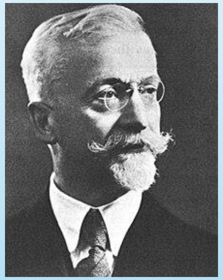
Information entropy

Formulation of quantum thermodynamics is under investigation.....

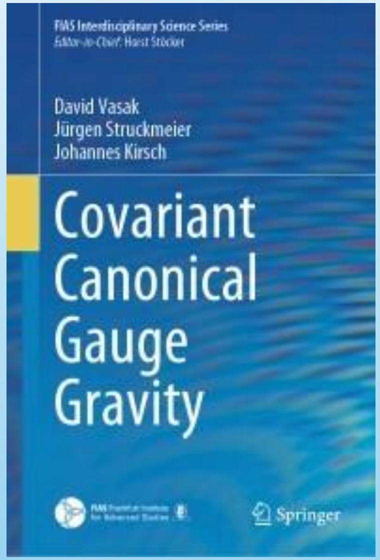
Thermodynamics in (modified) gravity



Gravity = Curvature + Torsion



Dark matter,
Dark energy, ...

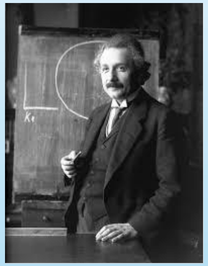


Free diffusion (Brownian motion)

Flat space without torsion $\partial_t \rho = \nu \Delta \rho$

Curved space with torsion $\partial_t \rho = -\nabla_i \left(\rho(\nu g^{ij} K^k{}_{jk}) \right) + \nu g^{ij} \nabla_i \nabla_j \rho$ $\nabla_i u^j = \partial_i u^j + \begin{Bmatrix} j \\ ki \end{Bmatrix} u^k + K^j{}_{ki} u^k$

Thermodynamics in (modified) gravity



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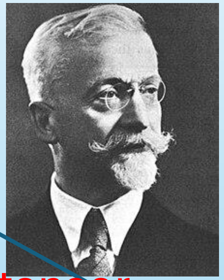

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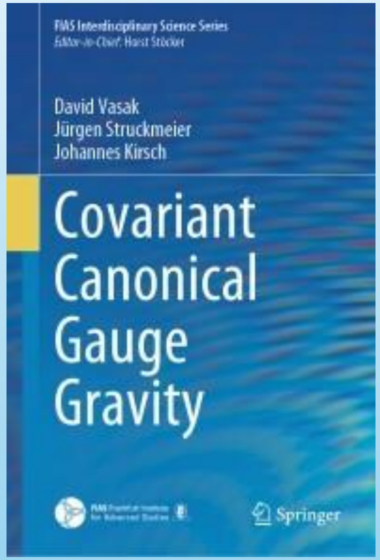

Contorsion tensor

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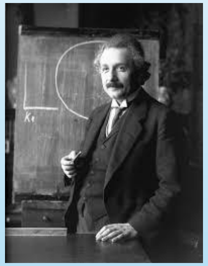

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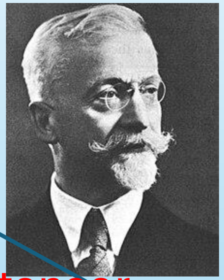

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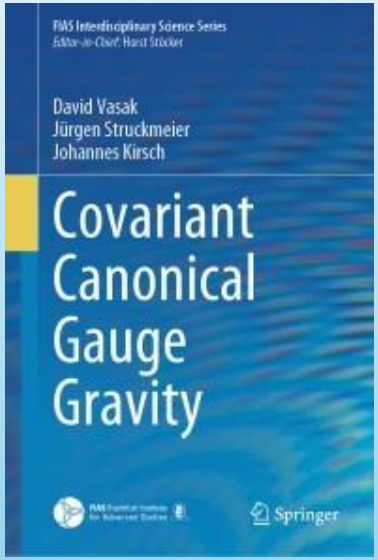

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1. Torsion (vierbein) is considered exclusively associated with the spin degrees of freedom. However, it is also noteworthy that we cannot avoid introducing vierbein to construct Brownian motion in generalized coordinates.
2. One way to study thermodynamical behavior in curved (spacetime) geometry with or without torsion, is to consider Brownian motion.
3. Is it possible to construct stochastic and quantum thermodynamics in this case?

No torsion

Giordano, Eur. Phys. J. B 92, 174 (2019).

Thermodynamics and Universe

1) Expansion of universe

$T_{rad} \propto R^{-1}(t)$	$s_{rad} R^3 \sim R^3 T^3 = const$
$T_{mat} \propto R^{-2}(t)$	$S_{mat} \sim \ln\left(R^3 T^{3/2}\right) = const$

Different from the expansion of volume of gas

What is the non-equilibrium effect?

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2) Self gravitating system

Sakagami&Taruya,Contiuum Mech. Thermodyn. 16, 279 (2004)

Chavanis et al.,Phys.Rev.E66, 036105 (2002)

From the virial theorem,

$$\Delta T \sim \Delta E_{kin} = -\Delta E_{tot}$$

→ Heat capacity is negative

→ Thermo. inhomogeneity is enhanced.

→ gravitational contraction (collapse)

Can this be modeled using Brownian motion?
Fluctuation effect in self-gravitating systems?

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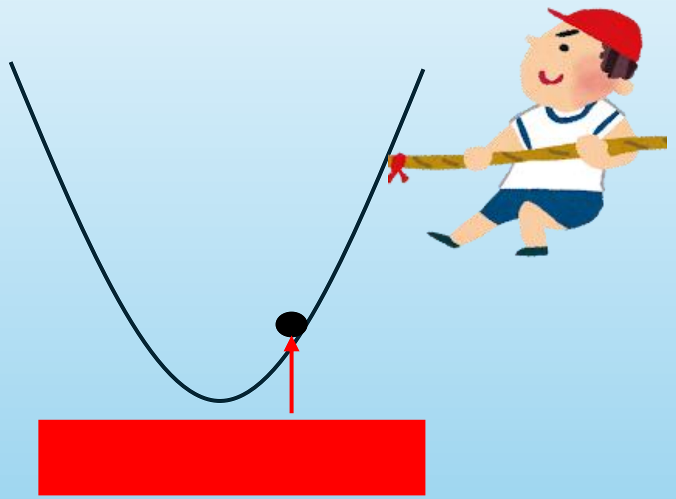
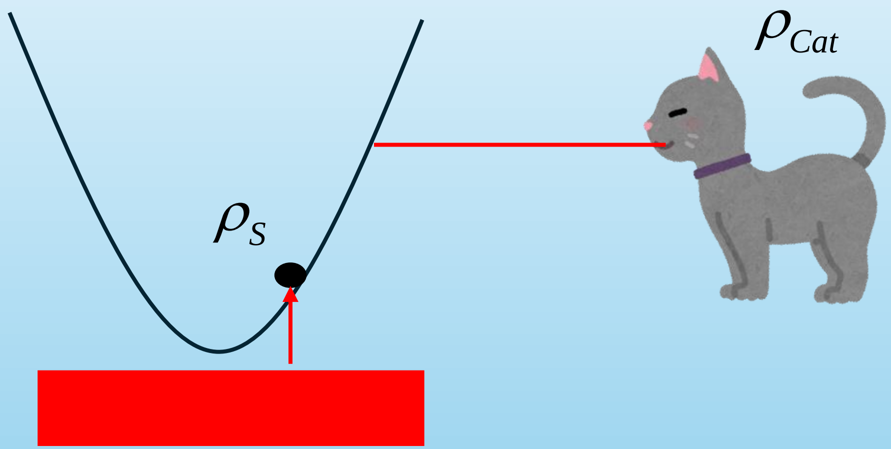
3) Brownian motion and Black Hole populations in globular clusters

Roupas, A&A 646 A20 (2021).
Chavanis&Mannella, Eur. Phys. J. B 78, 139 (2010).

4) Black hole and entropy

Thermo. work and Q. measurement





$$\rho_S \otimes \rho_{Cat} \Rightarrow U \rho_S \otimes \rho_{Cat} U^\dagger$$

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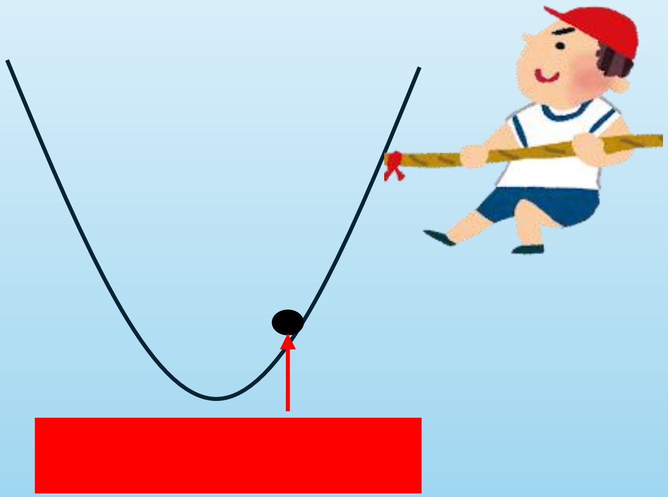

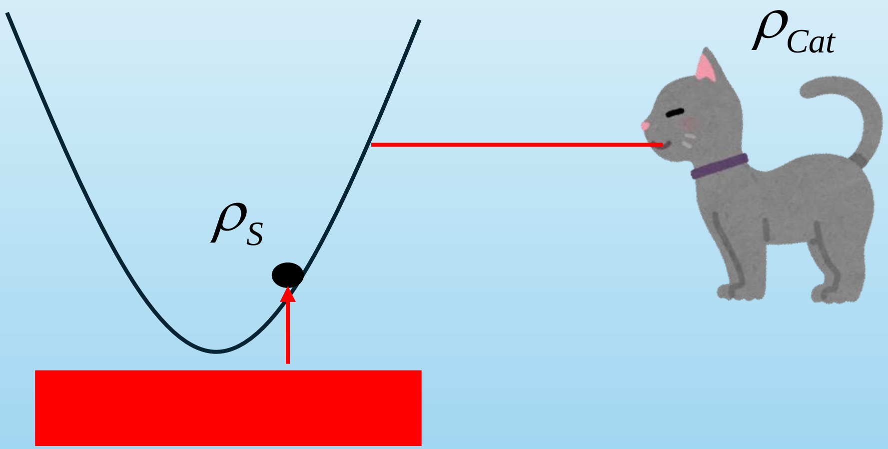

$$\rho_S \otimes \rho_{Cat} \Rightarrow U \rho_S \otimes \rho_{Cat} U^\dagger$$

1. What is the relation between classical and quantum optimal controls for external perturbation?

Sekimoto&Sasa, J. Phys. Soc. Japan, 66, 3658 (2001)
Schmiedl&Seifert, Phys. Rev. Lett. 98, 108301 (2007)
Koide, J. Phys. A50, 325001 (2017, Berry's phase)

?????

2. What is the role of quantum measurement (Maxwell Deamon) and what is its classical limit?

Classical limit?

Scully et al., Science 299, 862 (2003).
Kammerlander&Anders, Scientific reports 6, 22174 (2016).
Elouard et al., Phys. Rev. Lett. 118, 260603 (2017).

TUR (thermodynamical uncertainty relations)

Barato&Seifert, PRL114, 158101 (2015)   Hasagawa&Van Vu, PRL123,20001 (2017)

1. A particle trajectory in a nonequilibrium steady state Γ
2. An observable ϕ satisfying $\phi\left(\Gamma^{TR}\right)=-\phi\left(\Gamma\right)$
3. The probability distribution of the trajectories $P(s,\phi)$
4. The fluctuation theorem $\dfrac{P(s,\phi)}{P(-s,-\phi)}=e^{s}$

Time reversed trajectory

Entropy production

TUR $$\frac{\left\langle\left(\phi-\langle\phi\rangle\right)^2\right\rangle}{\langle\phi\rangle^2}\geq\frac{2}{e^{\sigma\tau}-1}$$

$$\langle s\rangle=\sigma\tau$$

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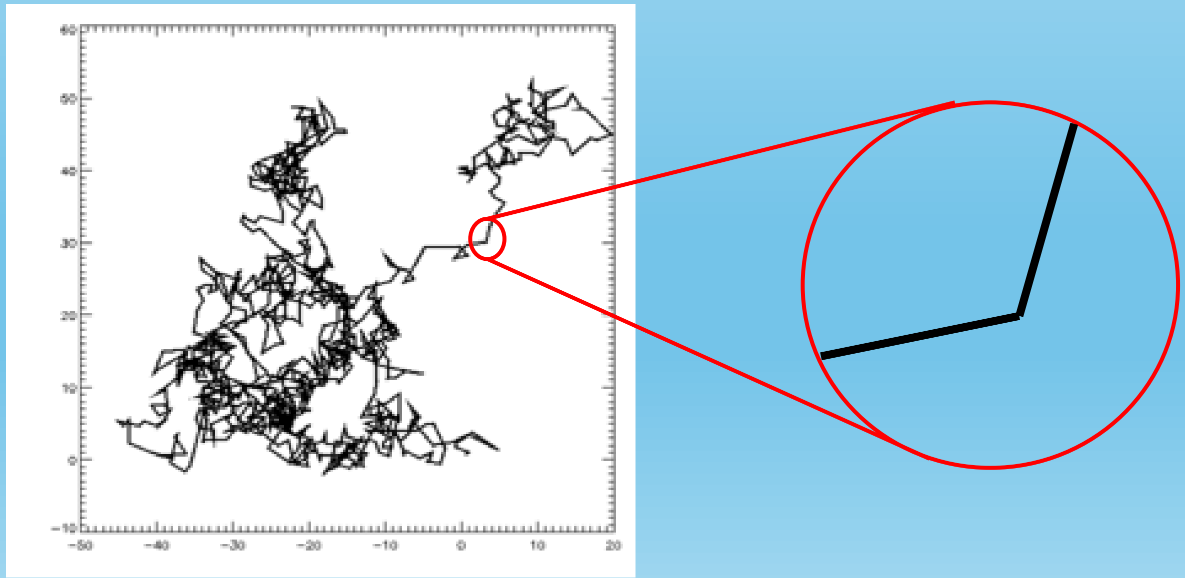


Is there TUR induced by non-differentianility?

de Matos et al., WATER12,3263 (2020)

Furthermore.....

$$\eta_{Car} = 1 - \frac{T_c}{T_h} \quad \eta_{CA} = 1 - \sqrt{\frac{T_c}{T_h}}$$

1. Efficiency of heat engine in finite-time operations (Cruzon-Ahlborn efficiency, Am. J. Phys. 43, 22, 1975)

2. How can we take the thermodynamical limit in stochastic and quantum thermodynamics?

3. Finite chemical potential? (Neidig,et al., arXiv:2308.07659)

4. Relation between the GKSL equation and the quantization of damped HO

5. Entanglement in classical stochastic mechanics (Reciprocal process)? (Schrödinger, Akad.Phys.Math.Klasse 1,144 (1931), Koide, J. Phys. Commun. 2, 021001 (2018))

Concluding remarks

1. We develop a general model of Brownian motion in flat spacetime.

2. We can define heat and entropy so that the behaviors of the model are consistent with thermodynamics.

3. A quantum master equation is derived from the model by applying the canonical quantization.

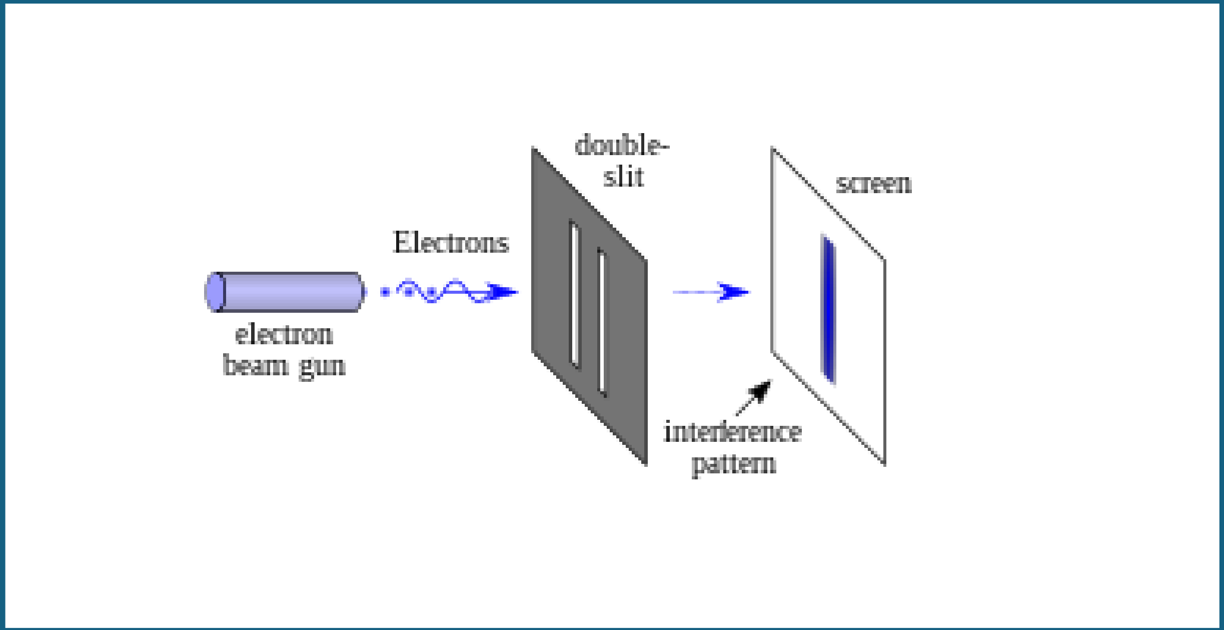
4. Given a system Hamiltonian, the form of our quantum master equation is determined except for a few parameters. (Advantage 1)

5. Regardless of the choice of the system Hamiltonian, the classical limit of the quantum master equation always describes a thermal relaxation process. (Advantage 2)

6. The derived master equation does not always satisfy the CPTP condition but, in several applications, we can find the parameters where the quantum master equation becomes a GKSL equation.

7. Our approach enables us formulate a unified framework of stochastic and quantum thermodynamics.

Let us consider the double-slit experiment.



1. The wave function of this system $\phi(\vec{x},t)$

2. Then we define a vector field by

$$\vec{u}(\vec{x},t)=\frac{\hbar}{m}\nabla\left\{\mathrm{Re}\left[\ln\phi(\vec{x},t)\right]+\mathrm{Im}\left[\ln\phi(\vec{x},t)\right]\right\}$$

The probability distribution is reproduced by the frequency distribution of Brownian motion,

Nelson, PR150,1079('66)

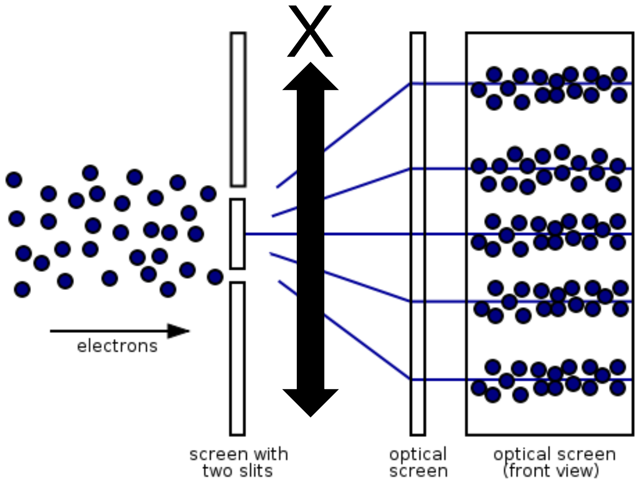
$$d\vec{r}(t) = \vec{u}(\vec{r}(t),t) + \sqrt{\frac{\hbar}{m}}\,d\vec{W}(t)$$

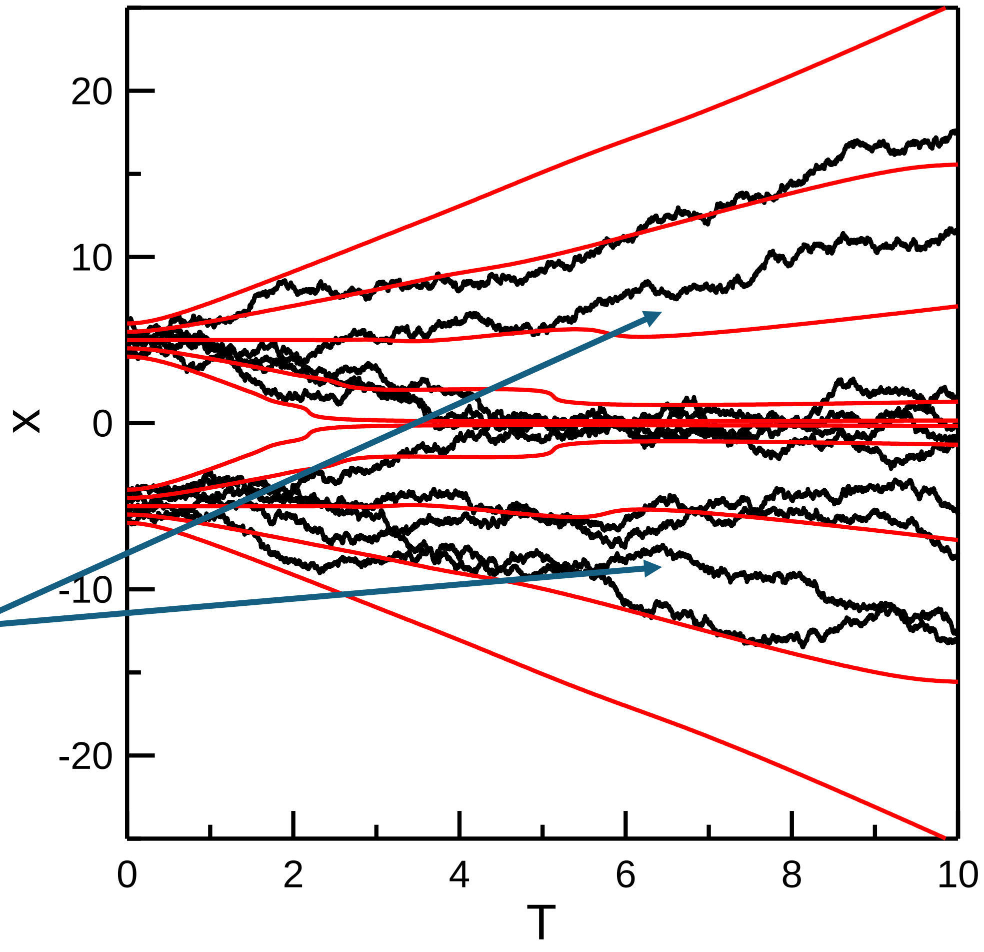
The position of a quantum particle

Planck constant

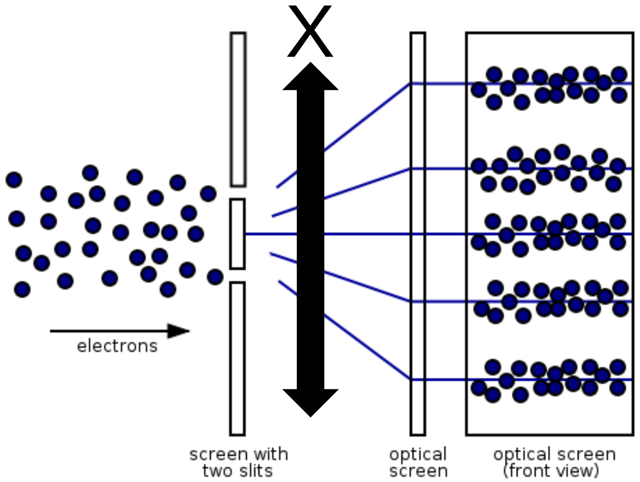
Gaussian white noise

$$\vec{u}(\vec{x},t) = \frac{\hbar}{m}\nabla\left\{\mathrm{Re}\left[\ln\phi(\vec{x},t)\right] + \mathrm{Im}\left[\ln\phi(\vec{x},t)\right]\right\}$$

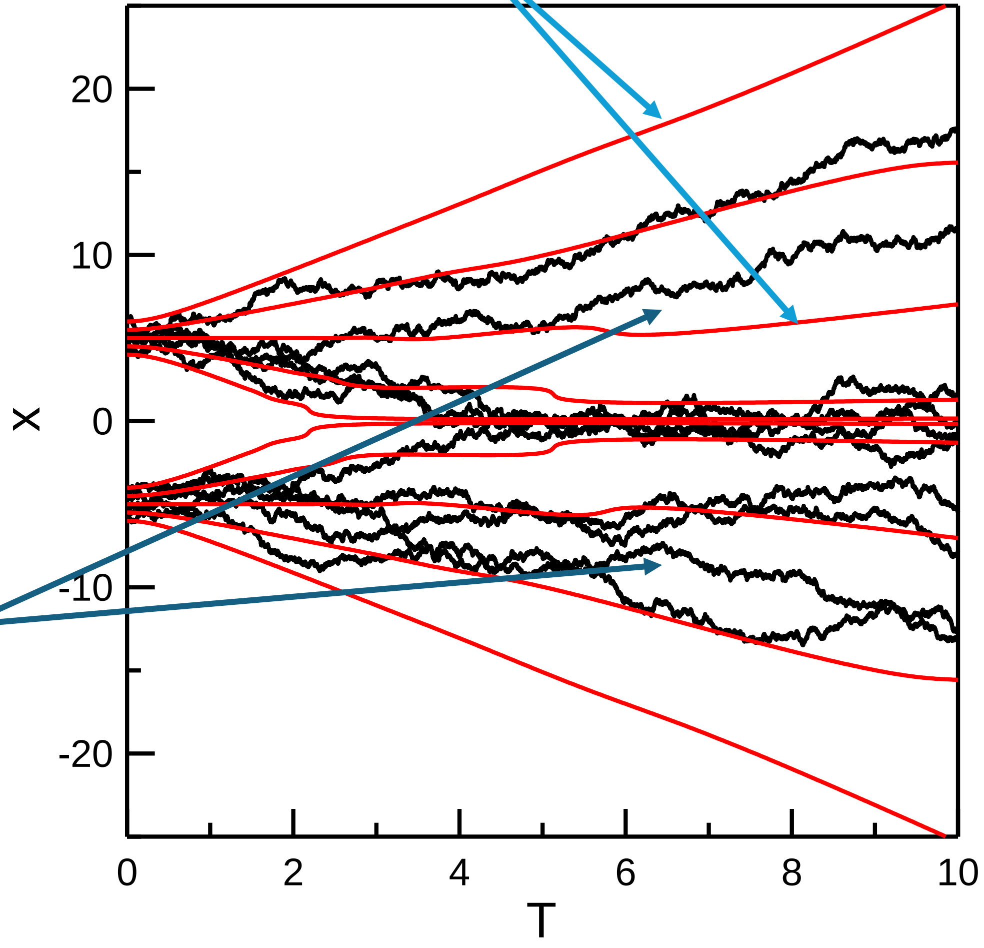




Brownian motion



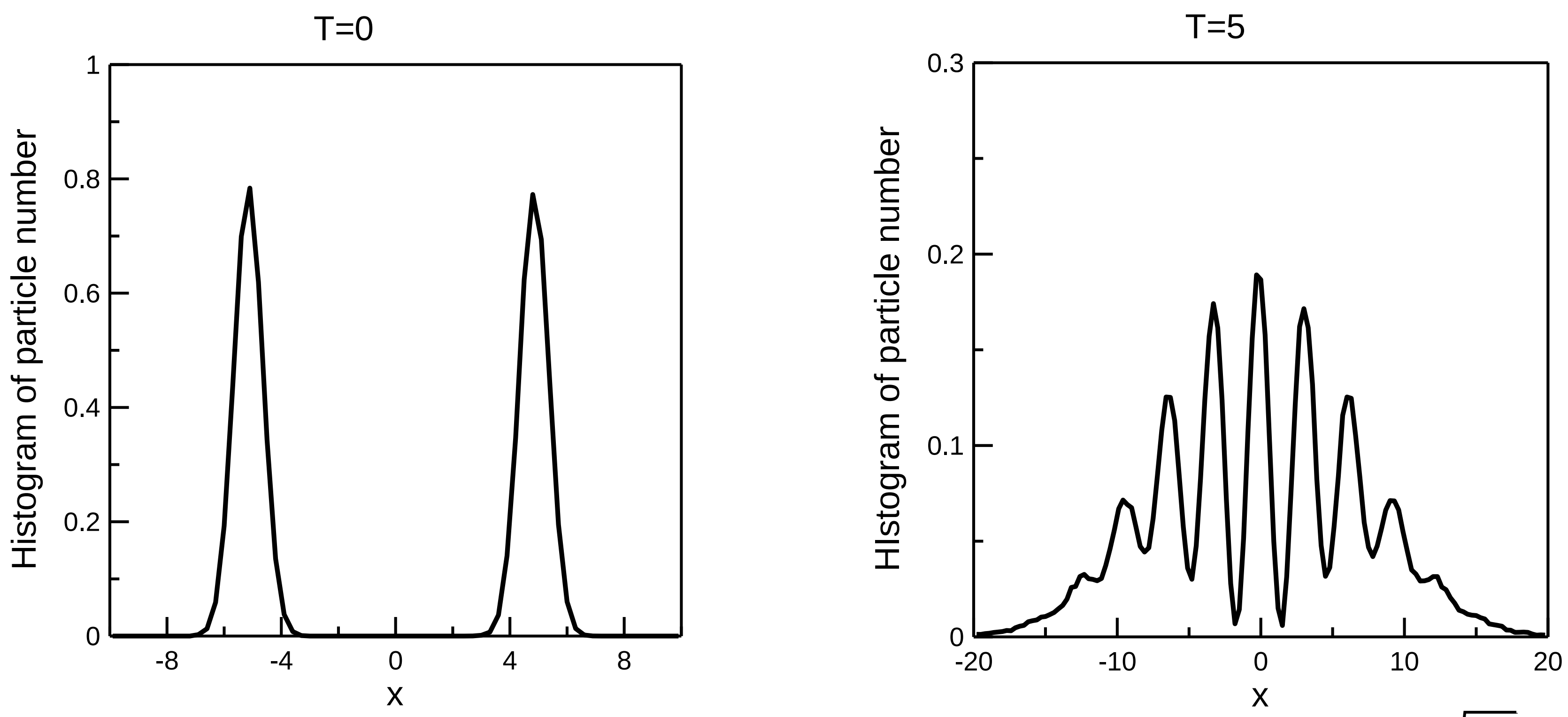
Bohmian trajectory



Brownian motion

200000 Brownian particles

5000 time steps



Simulation of $d\vec{r}(t) = \vec{u}(\vec{r}(t),t)dt + \sqrt{\frac{\hbar}{m}}d\vec{W}(t)$

200000 Brownian particles

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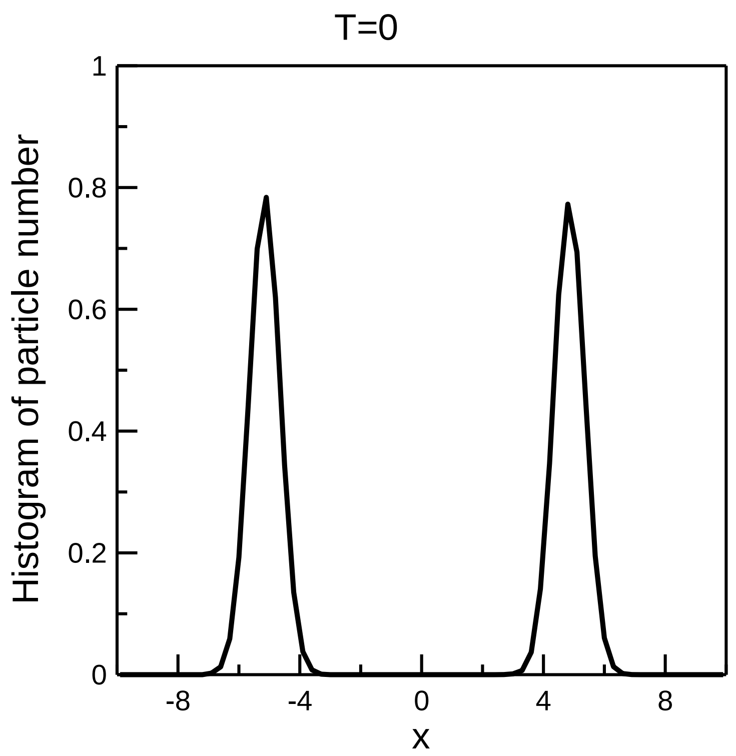
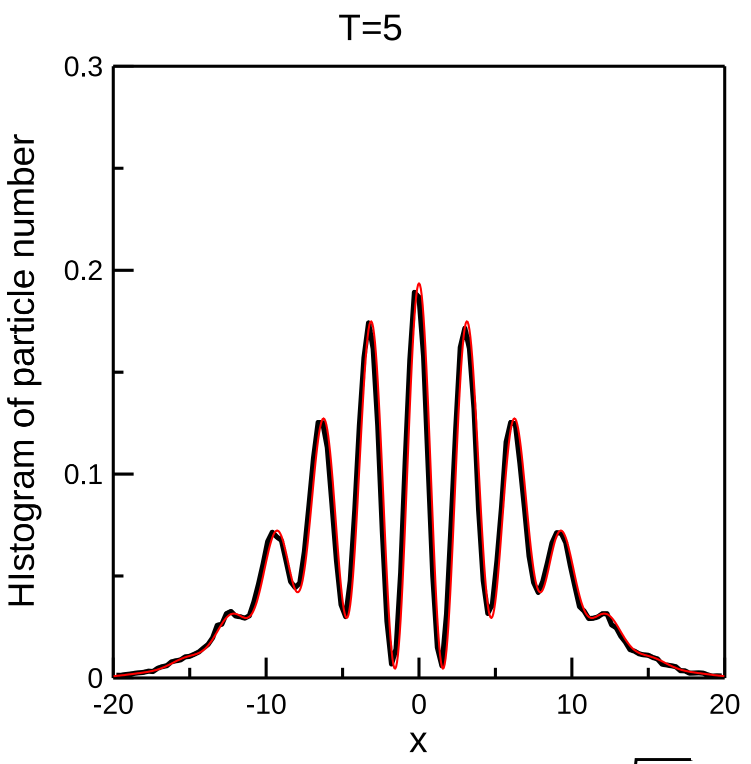
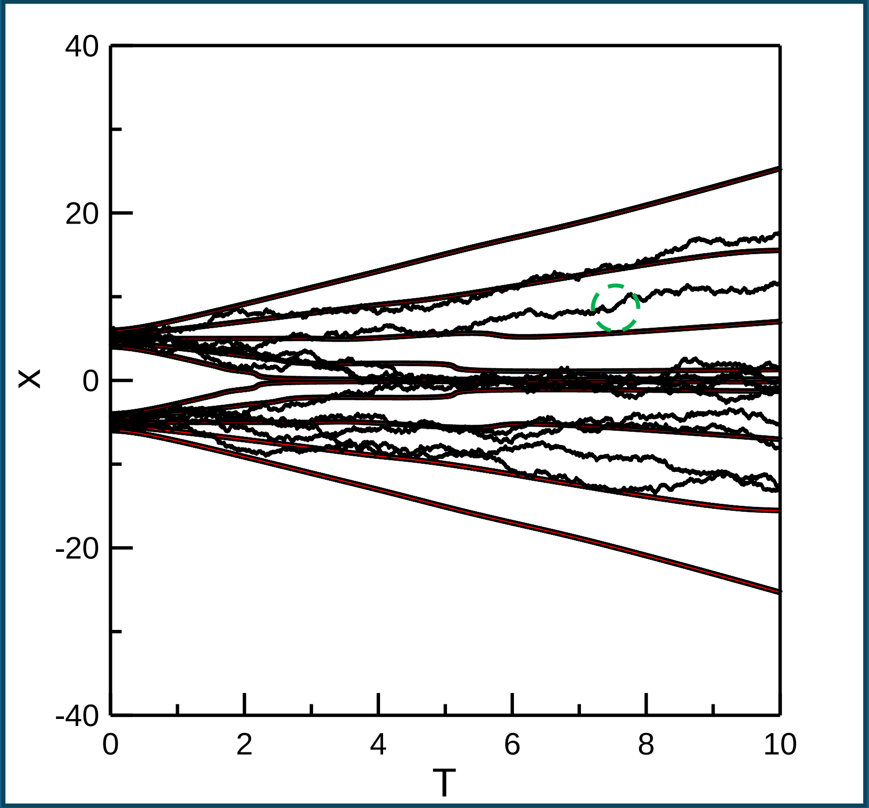


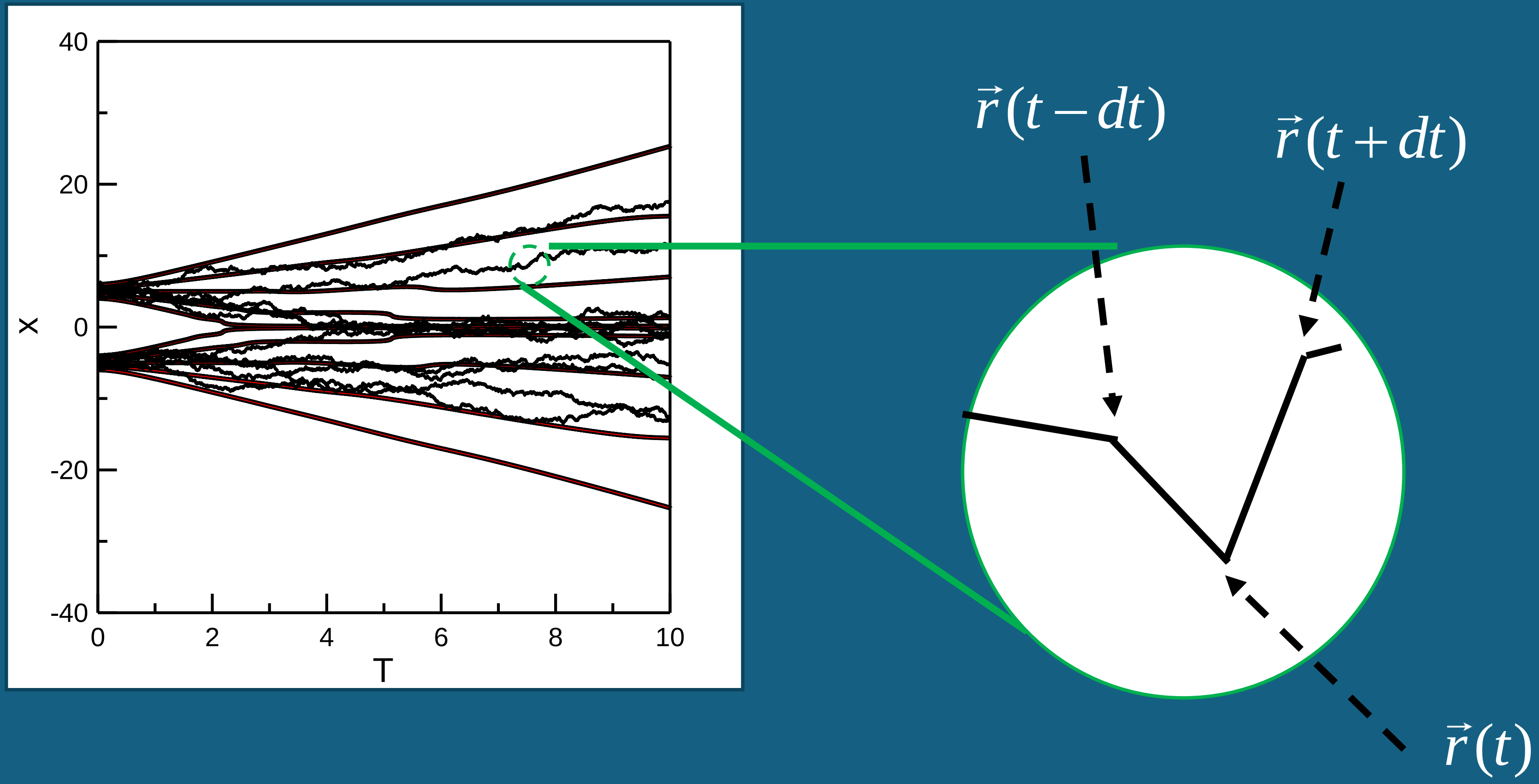


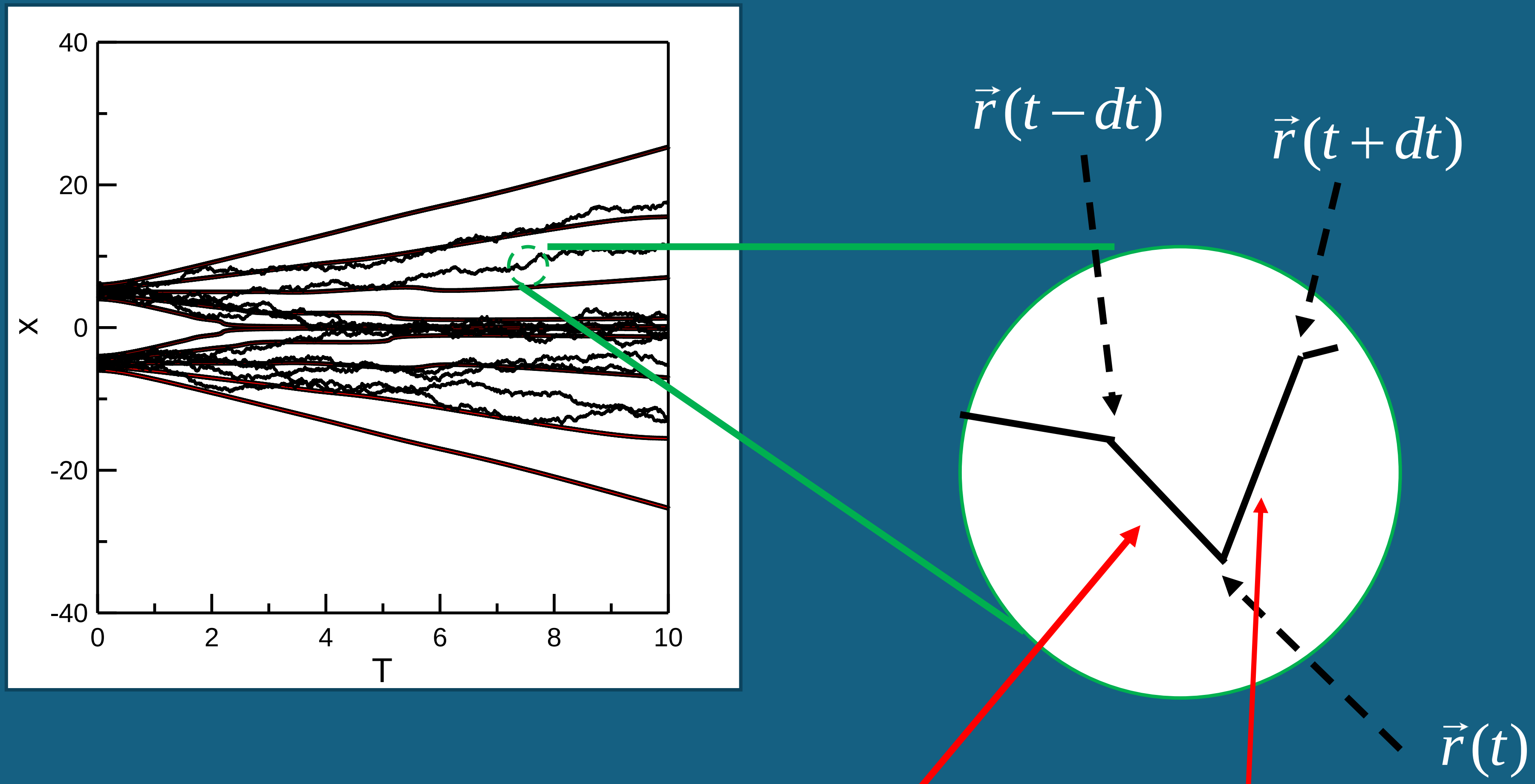
Simulation of $d\vec{r}(t) = \vec{u}(\vec{r}(t),t)dt + \sqrt{\frac{\hbar}{m}}d\vec{W}(t)$

Exact result

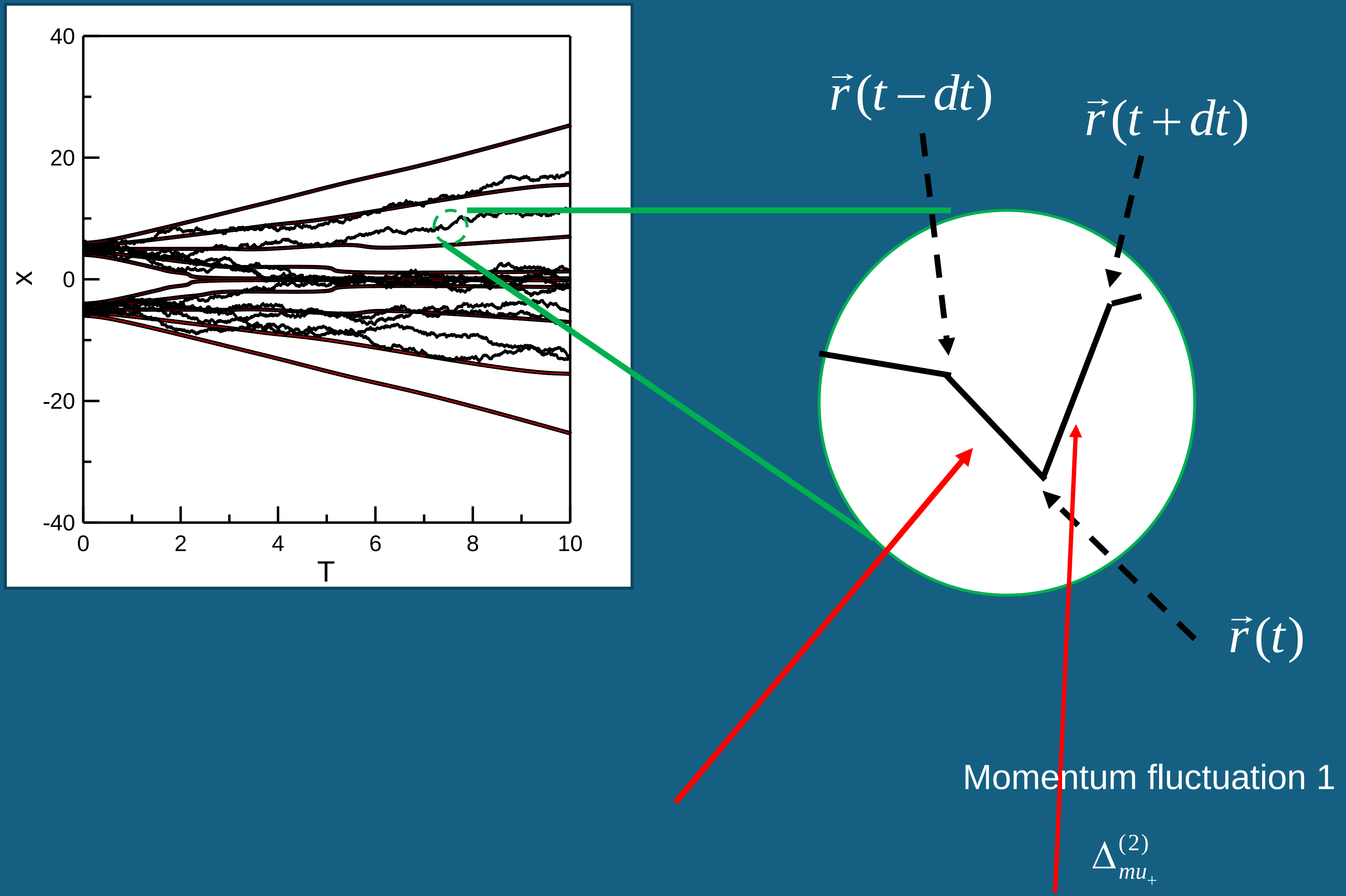


40
20
0
-20
-40
X
0
2
4
6
8
10
T


40
20
0
-20
-40
X
0
2
4
6
8
10
T
$\vec{r}(t-dt)$
$\vec{r}(t+dt)$
$\vec{r}(t)$



We can find, at least, two velocities.



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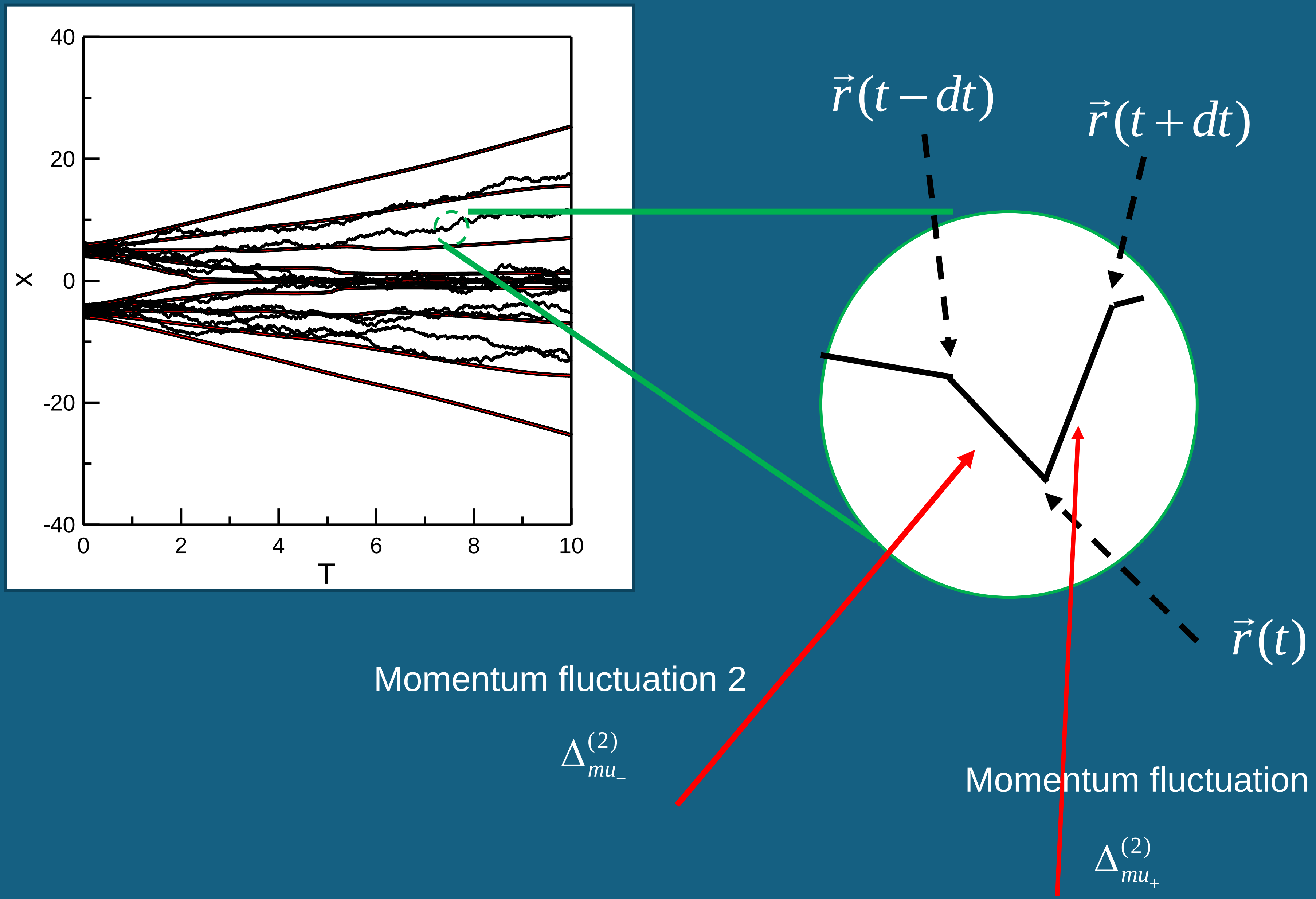

We can find, at least, two velocities.

Suppose that the fluctuation of the observed momentum is given by the average of the two fluctuations.

$$\Delta_p^{(2)} = \frac{\Delta_{mu_+}^{(2)} + \Delta_{mu_-}^{(2)}}{2}$$

Koide&Kodama, PLA382, 1472 ('18)

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$$\Delta_x^{(2)} \Delta_p^{(2)} \geq \frac{\hbar^2}{4}$$

The Kennard inequality in quantum mechanics

Koide&Kodama, PLA382, 1472 ('18)

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The Kennard inequality in quantum mechanics

The uncertainty relation can be induced from the non-differentiability of observables.

Koide&Kodama, PLA382, 1472 ('18)