Canonical Quantization of Brownian Motion and Quantum Thermodynamics

Tomoi Koide (IF UFRJ)
(collaboration with Fernando Nicacio (IF UFRJ))

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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)

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

Attempts to this generalization

- Classical side
- Quantal side

Small systems

Time evolutions from arbitrary states

Stochastic thermodynamics

Quantum thermodynamics

These formulations are yet under construction.
Stochastic Thermodynamics
Stochastic thermodynamics (stochastic energetics)

\[ dx_t = \frac{p_t}{m} \, dt \]
\[ dp_t = -\partial V(q_t, \lambda_t) \, dt \]
Stochastic thermodynamics (stochastic energetics)

\[
V(x, \lambda_t)
\]

External confinement potential

Interaction with heat bath

Heat bath of \( \beta^{-1} \)

Standard Brownian motion

\[
\begin{align*}
\dot{x}_t &= \frac{p_t}{m} dt \\
\dot{p}_t &= -\partial V(q_t, \lambda_t) dt
\end{align*}
\]
Stochastic thermodynamics (stochastic energetics)

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

Interaction with heat bath

1. dissipation
2. fluctuation

Heat bath of $\beta^{-1}$

Standard Brownian motion

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

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

Standard Wiener process (Gaussian white noise)
Stochastic thermodynamics (stochastic energetics)

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

\[ dQ^c_t = \int d\Gamma_0 f_0 (\Gamma_0) E \left[ \left( -\gamma \frac{p_t}{m} dt + \sqrt{\frac{2\gamma}{\beta}} \right) \circ dx_t \right] \]

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

\[ d\Gamma_0 = dq_0 dp_0 \]

\[ f_0 (\Gamma_0) : \text{initial phase space distribution} \]
Stochastic thermodynamics (stochastic energetics)


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

\[
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\]

\[E[\ldots] : \text{ensemble average for thermal fluctuation (Wiener)}\]

Energy

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

Work by heat bath

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

\[d\Gamma_0 = dq_0 dp_0 \quad f_0 (\Gamma_0) : \text{initial phase space distribution}\]
Stochastic thermodynamics (stochastic energetics)

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

First law

\[ U_{t_f}^c - U_{t_i}^c = dQ_t^c + dW_t^c \]

Energy

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

Work by heat bath

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

\[ d\Gamma_0 = dq_0 dp_0 \quad f_0 (\Gamma_0) : \text{initial phase space distribution} \]
Stochastic thermodynamics (stochastic energetics)


Information entropy

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

Second law

\[
\frac{dS_c}{dt} - k_B \beta \frac{dQ^c_t}{dt} \geq 0
\]

The equality is satisfied for the equilibrium distribution,

\[ f_{eq} = \frac{1}{Z} e^{-\beta \left( \frac{p^2}{2m} + V(x, \lambda) \right)} \]
Jarzynski equality

\[ \lambda_0 = a \]

\[ \lambda_1 = b \]

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

$$W_{0 \rightarrow 1}^c = \int d\Gamma_0 f_{eq} (\Gamma_0) E \left[ \int_0^1 d\tilde{W}_t^c \right]$$
Let us consider the external perturbation characterized by $\lambda_0 = a \rightarrow \lambda_1 = b$. Then the averaged work in this process is

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

Then, for the above process, we can show

Jarzynski equality

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

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

Jarzynski equality is one of fluctuation theorems.
Let us consider the external perturbation characterized by $\lambda_0 = a \rightarrow \lambda_1 = b$. Then the averaged work in this process is

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

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

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

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

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

3. Trace conservation
   \[ \text{Tr}[\hat{\rho}] = \text{Tr} \left[ M \left[ \hat{\rho} \right] \right] \]

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

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

\[
D[\hat{\rho}] = \sum_i \gamma_i \left\{ -\frac{1}{2}[\hat{L}^\dagger_i \hat{L}_i, \hat{\rho}] + \hat{L}_i \hat{\rho} \hat{L}_i^\dagger \right\}
\]

\( \gamma_i \geq 0 \) : 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
For the harmonic oscillator Hamiltonian, we can find the Lindblad operator which is consistent with thermodynamics:

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

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

\[ \gamma_- = e^{-\beta \hbar \omega} \]

\[ \gamma_+ \]

Detailed balance condition

Even if this is not satisfied, the equation is CPTP, but does not describe thermal equilibration.
For the harmonic oscillator Hamiltonian, we can find the Lindblad operator which is consistent with thermodynamics

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

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

\[ \gamma_- = e^{-\beta \hbar \omega} \quad \gamma_+ \]

Detailed balance condition

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

Quantum heat

\[ dQ_t^q := \text{Tr} \left[ \hat{H} d\hat{\rho}_t \right] \]

von Neumann entropy

\[ S_t^q := -k_B \text{Tr} \left[ \hat{\rho}_t \ln \hat{\rho}_t \right] \]

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......
Our strategy is......

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

1) propose

Brownian motion $\rightarrow$ Stochastic thermodynamics

CPTP evolution $\rightarrow$ Quantum thermodynamics
Our strategy is......

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

1) propose

Brownian motion

2) Thermodynamically consistent

Stochastic thermodynamics

CPTP evolution

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

1) propose  
2) Thermodynamically consistent

Our strategy is......

Brownian motion → Stochastic thermodynamics

CPTP evolution → Quantum thermodynamics

3) Canonical quantization
Generalized Brownian Motion
Generalized Brownian motion

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

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

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

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

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

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

\[
\begin{align*}
    dq_{(i)t} &= \frac{\partial H}{\partial p_{(i)t}} dt \\
    dp_{(i)t} &= -\frac{\partial H}{\partial q_{(i)t}} dt - \gamma_{qi} \frac{\partial H}{\partial p_{(i)t}} dt + \sqrt{\frac{2\gamma_{pi}}{\beta_i}} dB_{p(i)t}
\end{align*}
\]

\[
\begin{align*}
    E\left[ dB_{q(i)t}^{\alpha} dB_{q(j)t'}^{\beta} \right] &= E\left[ dB_{p(i)t}^{\alpha} dB_{p(j)t'}^{\beta} \right] = dt \delta_{ij} \delta_{\alpha\beta} \delta_{tt'} \\
    E\left[ dB_{q(i)t}^{\alpha} dB_{p(j)t'}^{\beta} \right] &= 0
\end{align*}
\]
Generalized Brownian motion


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

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

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

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

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

$$\mathbb{E}\left[ dB_{q(i)t}^\alpha dB_{p(j)t'}^\beta \right] = 0$$
Thermodynamical quantities


Energy

\[ U^c_t = \int d\Gamma_0 f_0 (\Gamma_0) E \left[ H(\Gamma_t, \lambda_t) \right] \]

Work

\[ dW^c_t = \int d\Gamma_0 f_0 (\Gamma_0) E \left[ d\tilde{W}^c_t \right] \quad d\tilde{W}^c_t := \frac{\partial H(\Gamma_t, \lambda_t)}{\partial \lambda_t} d\lambda_t \]

Heat

\[ dQ^c_{(i)t} = \int d\Gamma_0 f_0 (\Gamma_0) \sum_\alpha E \left[ \left( -\gamma_{p_i} \frac{\partial H}{\partial p^\alpha_{(i)t}} dt + \sqrt{\frac{2\gamma_{p_i}}{\beta_i}} dB^\alpha_{p(i)t} \right) \circ dq^\alpha_{(i)t} \right] \]

\[ -\int d\Gamma_0 f_0 (\Gamma_0) \sum_\alpha E \left[ \left( -\gamma_{q_i} \frac{\partial H}{\partial q^\alpha_{(i)t}} dt + \sqrt{\frac{2\gamma_{q_i}}{\beta_i}} dB^\alpha_{q(i)t} \right) \circ dp^\alpha_{(i)t} \right] \]

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.

Stochastic energetics

First law

\[
U_{t+dt}^c - U_t^c = \sum_i dQ_{(i)t}^c + dW_t^c
\]

Second law

\[
\frac{dS_t^c}{dt} - \sum_{i=1}^N k_B \beta_i^{-1} \frac{dQ_{(i)t}^c}{dt} \geq 0 \quad S_t^c = -k_B \int d\Gamma f(\Gamma, t) \ln f(\Gamma, t)
\]

We can still apply thermodynamical interpretations to this generalized BM.

Canonical quantization and new quantum master equation
Stochastic thermodynamics

Brownian motion

GKSL equation

Quantum thermodynamics

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

1) propose

2) Thermodynamically consistent

Our strategy is......

3) Canonical quantization

Brownian motion → Stochastic thermodynamics

GKSL equation → Quantum thermodynamics

Apply quantization to phase space distribution.
The phase space distribution

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

\[
\alpha : \text{Components of vectors}
\]

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

\[
\partial_t f = -\{ f, H \}_PB + \sum_{i=1}^N \sum_{\alpha=1}^D \frac{\gamma p_i}{\beta_i} \left\{ e^{-\beta_i H} \left\{ e^{\beta_i H} f, q^{\alpha}_{(i)} \right\}_PB, q^{\alpha}_{(i)} \right\}_PB
\]

\[
+ \sum_{i=1}^N \sum_{\alpha=1}^D \frac{\gamma q_i}{\beta_i} \left\{ e^{-\beta_i H} \left\{ e^{\beta_i H} f, p^{\alpha}_{(i)} \right\}_PB, p^{\alpha}_{(i)} \right\}_PB
\]

\[
\{ g, h \}_PB = \sum_{i=1}^N \sum_{\alpha=1}^D \left( \frac{\partial g}{\partial q_i^\alpha} \frac{\partial h}{\partial p_i^\alpha} - \frac{\partial g}{\partial p_i^\alpha} \frac{\partial h}{\partial q_i^\alpha} \right)
\]
Canonical quantization

\[ \{g, h\}_{PB} \]

\[ f(\Gamma, t) \]

\[ e^{\pm \beta_i H} f(\Gamma, t) \]

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

\[ \hat{\rho}(t) \]

\[ e^{\pm \beta_i \hat{H}/2} \hat{\rho}(t) e^{\mp \beta_i \hat{H}/2} \]

New quantum master equation

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

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

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

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

\[ \frac{d \hat{\rho}_{eq}}{dt} = 0 \quad \hat{\rho}_{eq} = \frac{1}{Z} e^{-\beta \hat{H}} \]

Is this time evolution CPTP?


Let us consider a harmonic oscillator,

\[ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2} \omega^2 \hat{q}^2 \]

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

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

\[ \hat{L}_3 = \sqrt{\delta} \hat{q} \]

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

\[ \Gamma_i = \sqrt{(\delta + 2) \gamma_p e^{-\gamma_p \omega t}} \]

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

\[ D[\hat{\rho}] \rightarrow -\frac{1}{2\hbar} \sum_{\mu \nu = 1}^{4} \eta_{\mu \nu} \left\{ \left[ \hat{L}_\mu \hat{L}_\nu, \hat{\rho} \right] + 2 \hat{L}_\mu \hat{\rho} \hat{L}_\nu^\dagger \right\} \quad \eta_{\mu \nu} = \text{Diag}(1,1,1,-1) \]
Is this time evolution CPTP?

Let us consider a harmonic oscillator, 

\[ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2} \omega^2 \hat{q}^2 \]

violates CPTP

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


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

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

\[
\hat{L}_+ = \left( \hat{q} + \frac{i}{m\omega} \hat{p} \right) \quad \hat{L}_- = \left( \hat{q} - \frac{i}{m\omega} \hat{p} \right)
\]

\[
\gamma_+ = e^{\beta\hbar\omega/2} \frac{\gamma_p}{2\hbar\beta} \quad \gamma_- = e^{-\beta\hbar\omega} \quad \frac{\gamma_-}{\gamma_+}
\]

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

GKSL equation \quad \rightarrow \quad CPTP, but not always converges toward equilibrium

Our master equation \quad \rightarrow \quad Not always CPTP, but converges toward equilibrium
CPTP even in other interactions?

Nicacio & Koide in preparation.

\[
\hat{H} = \sum_{i=1}^{2} \left( \frac{\hat{p}_i^2}{2m} + \frac{m}{2} \omega_i^2 \hat{q}_i^2 \right) + \frac{K}{2} \left( \hat{q}_1 - \hat{q}_2 \right)^2 \\
m = \omega^{-1} \\
K = \omega
\]
CPTP even in other interactions?

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

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

Model for heat conduction (network model)

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

\[m = \omega^{-1}, \quad K = \omega\]

Nicacio & Koide in preparation.
Other topics
Stochastic energetics in Field theory

Brownian motion for the scalar field

\[
\begin{align*}
    d\phi(x_i,t) &= (dt) \frac{\delta H}{\delta \Pi(x_i,t)} - (dt)\gamma_\phi \frac{\delta H}{\delta \phi(x_i,t)} + \sqrt{\frac{2\gamma_\phi}{(dx)\beta}} dB^\phi(x_i,t) \\
    d\Pi(x_i,t) &= -(dt) \frac{\delta H}{\delta \phi(x_i,t)} - (dt)\gamma_\Pi \frac{\delta H}{\delta \Pi(x_i,t)} + \sqrt{\frac{2\gamma_\Pi}{(dx)\beta}} dB^\Pi(x_i,t)
\end{align*}
\]
Brownian motion for the scalar field

\[
\begin{align*}
    d\phi(x_i, t) &= (dt) \frac{\delta H}{\delta \Pi(x_i, t)} - (dt) \gamma_\phi \frac{\delta H}{\delta \phi(x_i, t)} + \sqrt{2 \gamma_\phi} dB^\phi(x_i, t) \\
    d\Pi(x_i, t) &= -(dt) \frac{\delta H}{\delta \phi(x_i, t)} - (dt) \gamma_\Pi \frac{\delta H}{\delta \Pi(x_i, t)} + \sqrt{2 \gamma_\Pi} dB^\Pi(x_i, t)
\end{align*}
\]

Heat

\[
\begin{align*}
    dQ_i^{sf} &= \int dx \left( -\gamma_\Pi \frac{\delta H}{\delta \Pi} + \sqrt{2 \gamma_\Pi} \frac{dB^\Pi}{dx} \right) \circ d\phi - \int dx \left( -\gamma_\phi \frac{\delta H}{\delta \phi} + \sqrt{2 \gamma_\phi} \frac{dB^\phi}{dx} \right) \circ d\Pi
\end{align*}
\]

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

Free diffusion (Brownian motion)

\[ \partial_i \rho = v \Delta \rho \]

Flat space without torsion

Curved space with torsion

\[ \partial_i \rho = -\nabla_i \left( \rho (\nabla g^{ij} K_{jk}^k ) \right) + \nabla g^{ij} \nabla_i \nabla_j \rho \]

\[ \nabla_i u^i = \partial_i u^i + \left\{ j \atop ki \right\} u^k + K_{jk}^i u^k \]

Dark matter, Dark energy, ...
Thermodynamics in (modified) gravity

Gravity = Curvature + Torsion

Free diffusion (Brownian motion)

Flat space without torsion

Curved space with torsion

\[ \partial_i \rho = \nabla_i \left( \rho \left( \nu \, g^{jk} K_{jk}^k \right) \right) + \nu \, g^{ij} \nabla_i \nabla_j \rho \]

\[ \nabla_i u^i = \partial_i u^j + \left\{ J_{\ell i} \right\} \, u^k + K_{\ell i}^j u^k \]

Contorsion tensor

Dark matter, Dark energy, ...
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?

1) Expansion of universe

\[
\begin{align*}
T_{rad} &\propto R^{-1}(t) & S_{rad}R^3 &\sim R^3T^3 = \text{const} \\
T_{mat} &\propto R^{-2}(t) & S_{mat} &\sim \ln\left(R^3T^{3/2}\right) = \text{const}
\end{align*}
\]

Different from the expansion of volume of gas

What is the non-equilibrium effect?
Thermodynamics and Universe

1) Expansion of universe

\[
\begin{align*}
T_{\text{rad}} & \propto R^{-1}(t) \\
T_{\text{mat}} & \propto R^{-2}(t) \\
S_{\text{rad}} R^3 & \sim R^3 T^3 = \text{const} \\
S_{\text{mat}} & \sim \ln\left( R^3 T^{3/2} \right) = \text{const}
\end{align*}
\]

Different from the expansion of volume of gas

What is the non-equilibrium effect?

Can this be modeled using Brownian motion?

From the virial theorem,

\[
\Delta T \sim \Delta E_{\text{kin}} = -\Delta E_{\text{tot}}
\]

Heat capacity is negative

Thermo. inhomogeneity is enhanced.

gravitational contraction (collapse)

2) Self gravitating system

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


4) Black hole and entropy
Thermo. work and Q. measurement

\[ \rho_S \otimes \rho_{\text{Cat}} \Rightarrow U \rho_S \otimes \rho_{\text{Cat}} U^\dagger \]
Thermo. work and Q. measurement

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

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

\[ \rho_S \otimes \rho_{\text{Cat}} \Rightarrow U \rho_S \otimes \rho_{\text{Cat}} U^\dagger \]

Classical limit?

TUR (thermodynamical uncertainty relations)


1. A particle trajectory in a nonequilibrium steady state

2. An observable $\phi$ satisfying $\phi(\Gamma^{TR}) = -\phi(\Gamma)$

3. The probability distribution of the trajectories $P(s,\phi)$

4. The fluctuation theorem $\frac{P(s,\phi)}{P(-s,-\phi)} = e^s$

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

Entropy production

$\langle s \rangle = \sigma \tau$
TUR (thermodynamical uncertainty relations)

1. A particle trajectory in a nonequilibrium steady state $\Gamma$

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4. The fluctuation theorem $\frac{P(s, \phi)}{P(-s, -\phi)} = e^s$

$\Gamma^{TR}$ is the time reversed trajectory.

The probability distribution $P(s, \phi)$ satisfies the fluctuation theorem.

The TUR is given by

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

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

Is there TUR induced by non-differentianility?

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

\[ \eta_{\text{Car}} = 1 - \frac{T_c}{T_h} \quad \eta_{\text{CA}} = 1 - \frac{T_c}{\sqrt{T_h}} \]


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


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

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

$$\vec{u}(\vec{x}, t) = \frac{\hbar}{m} \nabla \left\{ \text{Re} \left[ \ln \phi(\vec{x}, t) \right] + \text{Im} \left[ \ln \phi(\vec{x}, t) \right] \right\}$$
The probability distribution is reproduced by the frequency distribution of Brownian motion,

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

The position of a quantum particle

Gaussian white noise

The position of a quantum particle

Planck constant

\[ \dot{u}(\dot{x}, t) = \frac{\hbar}{m} \nabla \{ \text{Re} \left[ \ln \phi(\dot{x}, t) \right] + \text{Im} \left[ \ln \phi(\dot{x}, t) \right] \} \]
Brownian motion
**Bohmian trajectory**

- Brownian motion

---

**Screen with two slits**

- Optical screen

**X**
200000 Brownian particles

Simulation of\[ d\vec{r}(t) = \bar{u}(\vec{r}(t), t) dt + \sqrt{\frac{h}{m}} d\tilde{W}(t) \]

5000 time steps
200000 Brownian particles

Histogram of particle number
T=0

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

Exact result
We can find, at least, two velocities.
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Suppose that the fluctuation of the observed momentum is given by the average of the two fluctuations.

\[ \Delta_p^{(2)} = \frac{\Delta_{\mu_+}^{(2)} + \Delta_{\mu_-}^{(2)}}{2} \]
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\[ \Delta_{\mu}^{(2)} = \frac{\Delta_{\mu+}^{(2)} + \Delta_{\mu-}^{(2)}}{2} \]

\[ \Delta_{x}^{(2)} \Delta_{p}^{(2)} \geq \frac{\hbar^2}{4} \]

The Kennard inequality in quantum mechanics.
Suppose that the fluctuation of the observed momentum is given by the average of the two fluctuations.

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The Kennard inequality in quantum mechanics

\[ \Delta_{x}^{(2)} \Delta_{p}^{(2)} \geq \frac{\hbar^2}{4} \]

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

Koide&Kodama, PLA382, 1472 (‘18)