Path Integral Approach to Quantum Brownian Motion

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1. Quantum Brownian Motion
   - Path Integral Formalism
   - Product Initial State
   - General Initial State
   - Semiclassical Expansion

2. Use of Path Integrals in Classical Stochastic Systems
   - Martin-Siggia-Rose formalism
   - Classical Fluctuation Theorems from Symmetry of Generating Functionals

3. Summary and Outlook
   - Application to Quantum Fluctuation Theorems?

Quantum Brownian Motion: Caldeira-Leggett Model

Treat a heat bath as a collection of harmonic oscillators:

- System
$$H_S = \frac{p^2}{2m} + V(x, t)$$
- Bath
$$H_B = \sum_n \left(\frac{p_n^2}{2m_n} + \frac{1}{2} m_n \omega_n^2 q_n^2 \right)$$
- Interaction:
$$H_I = -x \sum_n \kappa_n q_n$$
- The interaction renormalises the potential, and we need counter term
$$H_C = \sum_n \frac{\kappa_n^2}{2 m_n \omega_n^2} x^2$$
- Total Hamiltonian $H = H_S + H_B + H_I + H_C$
$$H = \frac{p^2}{2m} + V(x, t) + \sum_n \left(\frac{p_n^2}{2m_n} + \frac{m_n \omega_n^2}{2} (q_n - \frac{\kappa_n}{m_n \omega_n^2} x)^2 \right)$$

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Path Integral Formalism for Reduced Density Matrix

- Time evolution of density matrix of the total system

$$\rho(t) = U(t,0)\rho(0)U^\dagger(t,0), \qquad U(t,0) = \mathbb{T}\exp(-\frac{i}{\hbar}\int_0^t H(t')dt')$$

- Matrix elements (with $q \equiv \{q_n\}$)

$$\begin{aligned}\rho(x_f, q_f; x_f', q_f'; t) &\equiv \langle x_f, q_f|\rho(t)|x_f', q_f'\rangle \\ &= \int dx_i \int dq_i \int dx_i' \int dq_i' \, \langle x_f, q_f|U(t,0)|x_i, q_i\rangle \\ &\quad \times \langle x_i, q_i|\rho(0)|x_i', q_i'\rangle\langle x_i', q_i'|U^\dagger(t,0)|x_f', q_f'\rangle\end{aligned}$$

- Reduced density matrix: Trace over bath

$$\rho_r(t) \equiv \mathrm{Tr}_B\rho(t), \qquad \rho_r(x_f, x_f'; t) = \int d q_f \, \rho(x_f, q_f; x_f', q_f; t)$$

- Path integral representation

$$\langle x_f, q_f | U(t,0) | x_i, q_i \rangle = \int_{x_i}^{x_f} \mathcal{D}x \int_{q_i}^{q_f} \mathcal{D}q \; e^{iS[x,q]/\hbar},$$

where the integral is over all paths $x(s)$, $q(s)$, $0 \le s \le t$ with $x(0) = x_i$, $x(t) = x_f$, $q(0) = q_i$ and $q(t) = q_f$.

- Total action $S[x,q] = S_S[x] + S_B[q] + S_{I,C}[x,q]$

$$S_S[x] = \int_0^t ds \left[\frac{m}{2} (\frac{dx}{ds})^2 - V(x(s), s) \right],$$

$$S_B[q] = \sum_n \int_0^t ds \left[\frac{m_n}{2} (\frac{dq_n}{ds})^2 - \frac{1}{2} m_n \omega_n^2 q_n^2(s) \right],$$

$$S_{I,C}[x,q] = \sum_n \int_0^t ds \left[\kappa_n q_n(s) x(s) - \frac{\kappa_n^2}{2 m_n \omega_n^2} x^2(s) \right]$$

- We have

$$\rho(x_f, q_f; x'_f, q'_f; t) = \int dx_i \int dq_i \int dx'_i \int dq'_i \times J(x_f, q_f, x'_f, q'_f; t|x_i, q_i, x'_i, q'_i; 0)\rho(x_i, q_i; x'_i, q'_i; 0)$$

where

$$J(x_f, q_f, x'_f, q'_f; t|x_i, q_i, x'_i, q'_i; 0) = \int_{x_i}^{x_f} \mathcal{D}x \int_{q_i}^{q_f} \mathcal{D}q \int_{x'_i}^{x'_f} \mathcal{D}x' \int_{q'_i}^{q'_f} \mathcal{D}q' \times \exp[\frac{i}{\hbar}(S[x, q] - S[x', q'])]$$

Product Initial State

- Suppose at $t = 0$

$$\rho(0) = \rho_S(0) \otimes \rho_B(0), \qquad \rho(x_i, q_i; x'_i, q'_i; 0) = \rho_S(x_i, x'_i; 0)\rho_B(q_i, q'_i; 0)$$

- Take

$$\rho_B(0) = e^{-\beta H_B}/Z_B, \qquad Z_B = \mathrm{Tr} e^{-\beta H_B}$$

- We have

$$\boxed{\rho_r(x_f, x'_f; t) = \int dx \int dx' \; J(x_f, x'_f, t|x_i, x'_i, 0)\rho_S(x_i, x'_i; 0)},$$

where

$$J(x_f, x'_f, t|x_i, x'_i, 0) = \int_{x_i}^{x_f} \mathcal{D}x \int_{x'_i}^{x'_f} \mathcal{D}x' \times \exp[\frac{i}{\hbar}(S_S[x] - S_S[x'] + S_{IF}[x, x'])]$$

- The influence functional

$$\exp[\frac{i}{\hbar}S_{IF}[x,x']] = \int dq_f \int dq_i \int dq'_i \int_{q_i}^{q_f} \mathcal{D}q \int_{q'_i}^{q_f} \mathcal{D}q' \; \rho_B(q_i, q'_i)$$
$$\times \exp[\frac{i}{\hbar}(S_B[q] + S_{I,C}[x,q] - S_B[q'] - S_{I,C}[x',q'])]$$

which can obtained after the integration over the bath variables.

- Note that

$$\rho_B(\{q\},\{q'\}) = \prod_n \frac{1}{Z_{B,n}} \int_{\bar{q}_n(0)=q'_{n,i}}^{\bar{q}_n(\hbar\beta)=q_{n,i}} \mathcal{D}\bar{q}_n \; e^{-S^E[\bar{q}_n]/\hbar}$$

where the Euclidean action is

$$S^E[\bar{q}_n] = \int_0^{\hbar\beta} ds \; \left\{ \frac{1}{2} m_n (\frac{d\bar{q}_n}{ds})^2 + \frac{1}{2} m_n \omega_n^2 \bar{q}_n^2(s)) \right\}$$

- The result of Gaussian path integral is

$$\rho_B(\{q\},\{q'\}) = \prod_n \frac{1}{Z_{B,n}} \left(\frac{m_n\omega_n}{2\pi\hbar \sinh(\beta\hbar\omega_n)} \right)^{1/2}$$
$$\times \exp\left[-\frac{m_n\omega_n}{2\hbar\sinh(\beta\hbar\omega_n)} \{(q_{n,i}^2 + q_{n,i}'^2)\cosh(\beta\hbar\omega_n) - 2q_{n,i}q'_{n,i}\} \right]$$

with

$$Z_B = \prod_n \left(\frac{1}{2\sinh(\beta\hbar\omega_n/2)} \right)$$

- Inserting this into expression for S_{IF}, we note that the remaining path integrals are all Gaussian. We can integrate explicitly over $\mathcal{D}q_n$ and $\mathcal{D}q'_n$ and then over the endpoints $q_{n,i}$, $q'_{n,i}$ and $q_{n,f}$. The result is as follows.

$$S_{IF}[x,x'] = i\int_0^t ds \int_0^s du\, (x(s)-x'(s))\{K(s-u)x(u) - K^*(s-u)x'(u)\}$$
$$-\frac{\mu}{2}\int_0^t ds\, (x^2(s) - x'^2(s))$$

where

$$\mu \equiv \sum_n \frac{\kappa_n^2}{m_n\omega_n^2}$$

$$K(s) \equiv \sum_n \frac{\kappa_n^2}{2m_n\omega_n} \frac{\cosh(\frac{1}{2}\beta\hbar\omega_n - i\omega_n s)}{\sinh(\frac{1}{2}\beta\hbar\omega_n)} = N(s) - \frac{i}{2}D(s)$$

where

$$N(s) = \sum_n \frac{\kappa_n^2}{2m_n\omega_n}\coth(\frac{1}{2}\beta\hbar\omega_n)\cos(\omega_n s), \qquad D(s) = \sum_n \frac{\kappa_n^2}{m_n\omega_n}\sin(\omega_n s)$$

Note that $J(x_f, x_f', t|x_i, x_i', 0) = \exp(i\Phi[x, x']/\hbar)$, where

$$\Phi[x, x'] = S_S[x] - S_S[x'] + S_{IF}[x, x']$$
$$= \int_0^t ds \left[m\dot{x}_c(s)\dot{x}_q(s) - \left\{ V\left(x_c(s) + \frac{x_q(s)}{2}, s \right) - V\left(x_c(s) - \frac{x_q(s)}{2}, s \right) \right\} \right]$$
$$+ \frac{i}{2} \int_0^t ds \int_0^t du\, x_q(s) N(s-u) x_q(u) + \int_0^t ds \int_0^s du\, x_q(s) D(s-u) x_c(u)$$
$$- \mu \int_0^t ds\, x_c(s) x_q(s)$$

where

$$\boxed{x_q(s) \equiv x(s) - x'(s), \qquad x_c(s) \equiv \frac{1}{2}(x(s) + x'(s))}$$

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General Initial State

- More realistic initial state

$$\rho(0) = \sum_m O_S^m \, \rho_\beta \, O_S'^m$$

where O_S^m and $O_S'^m$ are operators acting on system space and

$$\rho_\beta = \frac{1}{Z_\beta} e^{-\beta H}, \qquad Z_\beta = \mathrm{Tr} e^{-\beta H}$$

is the canonical density matrix of the whole system at equilibrium.

- Example: $\rho(0) = \rho_\beta$
- Example: Measurement at $t = 0^-$ on the system at equilibrium changes ρ_β to

$$\rho(0) = P \rho_\beta P$$

Preparation Function

- We have

$$\rho(x_i, q_i; x_i', q_i'; 0) = \sum_m \int d\bar{x} \int d\bar{x}' \; \langle x_i | O_S^m | \bar{x} \rangle \langle \bar{x}, q_i | \rho_\beta | \bar{x}', q_i' \rangle \langle \bar{x}' | O_S'^m | x_i' \rangle$$
$$= \int d\bar{x} \int d\bar{x}' \; \lambda(x_i, \bar{x}; x_i', \bar{x}') \rho_\beta(\bar{x}, q_i; \bar{x}', q_i'),$$

where the preparation function

$$\lambda(x_i, \bar{x}; x_i', \bar{x}') \equiv \sum_m \langle x_i | O_S^m | \bar{x} \rangle \langle \bar{x}' | O_S'^m | x_i' \rangle$$

specifies the deviation of the initial state from equilibrium.

- First we use the Euclidean path integral to represent

$$\rho_\beta(\bar{x}, q_i; \bar{x}', q_i') = \frac{1}{Z_\beta} \int_{\bar{x}(0)=\bar{x}'}^{\bar{x}(\hbar\beta)=\bar{x}} \mathcal{D}\bar{x} \int_{\bar{q}(0)=q_i'}^{\bar{q}(\hbar\beta)=q_i} \mathcal{D}\bar{q}$$
$$\times \exp[-\frac{1}{\hbar}(S_S^E[\bar{x}] + S_B^E[\bar{q}] + S_{I,C}^E[\bar{x}, \bar{q}])]$$

- Insert this initial state into the evolution equation and trace over the bath variables to finally obtain the evolution equation for the reduced density matrix

$$\boxed{\rho_r(x_f, x_f'; t) = \int dx_i \int dx_i' \int d\bar{x} \int d\bar{x}'\; J(x_f, x_f', t|x_i, \bar{x}; x_i', \bar{x}', 0)\lambda(x_i, \bar{x}; x_i', \bar{x}')}$$

We have

$$J(x_f, x_f', t|x_i, \bar{x}, x_i', \bar{x}', 0) = \frac{1}{Z}\int_{x_i}^{x_f}\mathcal{D}x\int_{x_i'}^{x_f'}\mathcal{D}x'\int_{\bar{x}'}^{\bar{x}}\mathcal{D}\bar{x}$$
$$\times \exp\left[\frac{i}{\hbar}(S_S[x] - S_S[x']) - \frac{1}{\hbar}S_S^E[\bar{x}] - \frac{1}{\hbar}\Psi[x, x', \bar{x}]\right]$$

where

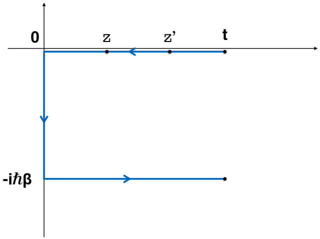
$$e^{-\Psi[x,x',\bar{x}]/\hbar} = \int dq_f \int dq_i \int dq_i' \; G[x](q_f, q_i) G^E[\bar{x}](q_i, q_i') G^*[x'](q_f, q_i')$$

with $1/Z \equiv Z_B/Z_\beta$ and

$$G[x](q_f, q_i) = \int_{q_i}^{q_f}\mathcal{D}q \; \exp[\frac{i}{\hbar}(S_B[q] + S_{I,C}[x, q])]$$
$$G^E[\bar{x}](q_i, q_i') = \frac{1}{Z_B}\int_{q_i'}^{q_i}\mathcal{D}\bar{q} \; \exp[-\frac{1}{\hbar}(S_B^E[\bar{q}] + S_{I,C}^E[\bar{x}, \bar{q}])]$$

After a lengthy calculation, one obtains

$$
\begin{aligned}
\Psi[x, x', \bar{x}] = & \int_0^t ds \int_0^s du\, (x(s) - x'(s))\{K(s-u)x(u) - K^*(s-u)x'(u)\} \\
& - i \int_0^t ds \int_0^{\beta\hbar} du\, K(-s-iu)(x(s) - x'(s))\bar{x}(u) \\
& - \int_0^{\beta\hbar} ds \int_0^s du\, K(-is+iu)\bar{x}(s)\bar{x}(u) \\
& + \frac{i}{2}\mu \int_0^t (x^2(s) - x'^2(s)) + \frac{\mu}{2} \int_0^{\beta\hbar} ds\, \bar{x}^2(s)
\end{aligned}
$$



$$\Psi[\tilde{x}] = \int dz \int_{z>z'} dz'\ K(z-z')\tilde{x}(z)\tilde{x}(z')$$

where

$$\tilde{x}(z) = \begin{cases} x'(s), & \text{if } z = s, \quad 0 \le s \le t \\ \bar{x}(s), & \text{if } z = -is, \quad 0 \le s \le \hbar\beta \\ x(s), & \text{if } z = s - i\hbar\beta, \quad 0 \le s \le t \end{cases}$$

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Expressions using x_q and x_c

- For convenience, look at only product initial state case. Recall

$$J(x_f, x_f', t|x_i, x_i', 0) = \int_{x_i}^{x_f} \mathcal{D}x \int_{x_i'}^{x_f'} \mathcal{D}x' \times \exp[\frac{i}{\hbar}(S_S[x] - S_S[x'] + S_{IF}[x, x'])]$$

- Change of variables: $x, x' \to x_q, x_c$, and $J(x_f, x_f', t|x_i, x_i', 0) \to J(x_{cf}, x_{qf}, t|x_{ci}, x_{qi}, 0)$. We can write

$$J(x_{cf}, x_{qf}, t|x_{ci}, x_{qi}, 0) = \int_{x_{qi}}^{x_{qf}} \mathcal{D}x_q \int_{x_{ci}}^{x_{cf}} \mathcal{D}x_c \ \exp[-\frac{1}{\hbar}\Sigma[x_c, x_q]]$$

- Recall that

$$S_{IF}[x,x'] = \frac{i}{2}\int_0^t ds\int_0^t du\; x_q(s)N(s-u)x_q(u)$$
$$+\int_0^t ds\int_0^s du\; x_q(s)D(s-u)x_c(u) - \mu\int_0^t ds\; x_q(s)x_c(s)$$

- We introduce damping kernel $\gamma(s)$ defined by

$$\boxed{D(s) \equiv -m\frac{d}{ds}\gamma(s)}, \qquad \boxed{\gamma(s) = \frac{1}{m}\sum_n \frac{\kappa_n^2}{m_n\omega_n^2}\cos(\omega_n s)}$$

- Integrating by parts,

$$\int_0^t ds\int_0^s du\; x_q(s)D(s-u)x_c(u) = -m\int_0^t ds\int_0^s du\; x_q(s)\gamma(s-u)\dot{x}_c(u)$$
$$- mx_c(0)\int_0^t ds\;\gamma(s)x_q(s) + m\gamma(0)\int_0^t ds\; x_q(s)x_c(s)$$

- The last term cancels those from the counter term, since

$$m\gamma(0) = \sum_n \frac{\kappa_n^2}{m_n \omega_n^2} = \mu$$

- We also have

$$S_S[x] - S_S[x'] = \int_0^t ds \, [m\dot{x}_q(s)\dot{x}_c(s) - V(x_c + \frac{x_q}{2}, s) + V(x_c - \frac{x_q}{2}, s)]$$

- We therefore have

$$\begin{aligned}\Sigma[x_c, x_q] =& \frac{1}{2} \int_0^t ds \int_0^t du \; x_q(s) N(s-u) x_q(u) \\ & - i \int_0^t ds \, [m\dot{x}_q(s)\dot{x}_c(s) - V(x_c + \frac{x_q}{2}, s) + V(x_c - \frac{x_q}{2}, s)] \\ & + im \int_0^t ds \int_0^s du \; x_q(s) \gamma(s-u) \dot{x}_c(u) + im x_c(0) \int_0^t ds \; \gamma(s) x_q(s)\end{aligned}$$

Classical Limit

- In the classical limit $\hbar \to 0$, the path integral is dominated by the paths for which Σ is stationary.
- Varying $x_q(s)$,

$$0 = m\ddot{x}_c(s) + \frac{\partial}{\partial x_q}\{V(x_c + \frac{x_q}{2}, s) - V(x_c - \frac{x_q}{2}, s)\}$$
$$+ m\int_0^s du\ \gamma(s-u)\dot{x}_c(u) + m x_{ci}\gamma(s) - i\int_0^t du\ N(s-u)x_q(u)$$

- Varying $x_c(s)$,

$$0 = m\ddot{x}_q(s) + \frac{\partial}{\partial x_c}\{V(x_c + \frac{x_q}{2}, s) - V(x_c - \frac{x_q}{2}, s)\}$$
$$- m\int_s^t du\ \gamma(u-s)\dot{x}_q(u)$$

- For the classical paths, we look for the case where $x_{qi} = x_{qf} = 0$ (no off-diagonal terms at initial and final times). Then the solution to saddle points equations is

$$x_q(s) = 0, \qquad 0 \leq s \leq t$$

- Classical path for x_c

$$m\ddot{x}_c(s) = -\frac{\partial}{\partial x_c} V(x_c, s) - m \int_0^s du\, \gamma(s-u)\dot{x}_c(u) - m x_{ci}\gamma(s)$$

- Appearance of x_{ci} term is due to the particular (product) initial state.

Semiclassical Expansion

- Consider fluctuation around $x_q(s) = 0$. Let

$$x_q(s) = \hbar y(s), \qquad x_c(s) = r(s)$$

- Note that in the limit $\hbar \to 0$,

$$\begin{aligned}\hbar N(s) =& \hbar \sum_n \frac{\kappa_n^2}{2m_n\omega_n} \coth(\frac{1}{2}\beta\hbar\omega_n) \cos(\omega_n s) \\ \to& \beta^{-1} \sum_n \frac{\kappa_n^2}{m_n\omega_n} \cos(\omega_n s) = \beta^{-1} m\gamma(s) \equiv \Gamma(s)\end{aligned}$$

- Then we can write

$$\begin{aligned}\frac{1}{\hbar}\Sigma[x_c, x_q] \simeq& \frac{1}{2}\int_0^t ds \int_0^t du\ y(s)\Gamma(s-u)y(u) \\ &+ i\int_0^t ds \left[y(s)\left\{ m\ddot{r}(s) + \partial_r V(r,s) + m\int_0^s du\ \gamma(s-u)\dot{r}(u) + mr(0)\gamma(s) \right\}\right] \\ \equiv& S_{cl}[r, y]\end{aligned}$$

- In this limit, we have

$$J(x_{cf}, x_{qf}, t|x_{ci}, x_{qi}, 0) \to J(r_f, t|r_i, 0) = \int_{y(0)=0}^{y(t)=0} \mathcal{D}y \int_{r(0)=r_i}^{r(t)=r_f} \mathcal{D}r \ \exp[-S_{cl}[r, y]]$$

with

$$\rho(r_f, t) = \int dr_i \ J(r_f, t|r_i, 0)\rho(r_i, 0)$$

- This action is just MSR action for classical stochastic equation

$$m\ddot{r}(s) + \partial_r V(r, s) + m\int_0^s du\, \gamma(s-u)\dot{r}(u) + mr(0)\gamma(s) = \xi(s)$$

where the noise $\xi(s)$ satisfies

$$\langle \xi(s) \rangle = 0, \qquad \langle \xi(s)\xi(s') \rangle = \Gamma(s-s')$$

- Classical FDR is represented by

$$m\gamma(s-s') = \beta\Theta(s-s')\Gamma(s-s')$$

MSR Formalism

- Consider a generalized Langevin equation (with a time-dep. protocal λ_t)

$$m\ddot{x}(t) + \partial_x V(x, \lambda_t) + m \int_0^t ds\, \gamma(t-s)\dot{x}(s) = \xi(t)$$

with a colored noise satisfying $\langle \xi(t) \rangle = 0$ and

$$\langle \xi(t)\xi(t') \rangle = \Gamma(t-t')$$

with $m\gamma(t-t') = \beta\Theta(t-t')\Gamma(t-t')$

- Distribution function $P_\xi[\xi]$ for noise

$$P_\xi[\xi] = (\text{const.}) \exp[-\frac{1}{2} \int dt \int dt'\ \xi(t) G(t-t')\xi(t')]$$

where

$$\int dt'\ G(t-t')\Gamma(t'-t'') = \delta(t-t'')$$

- The transition probability is

$$J(x_f, t|x_i, 0) = \int \mathcal{D}\xi \; P_\xi[\xi] \; \delta(x(t) - x_f),$$

where $x(t)$ is the solution to the Langevin equation with the initial condition $x(0) = x_i$.
- Use the identity

$$1 = \int \mathcal{D}x \; \delta(E[x](t) - \xi(t)) \; J,$$

where

$$E[x](t) = m\ddot{x}(t) + \partial_x V(x, \lambda_t) + m \int_0^t ds \; \gamma(t-s)\dot{x}(s)$$

and $J = \det[\delta E[x](t)/\delta x(t')]$ is the Jacobian, which is a constant indep. of x.
- Insert the integral representation of the delta-function,

$$1 = \int \mathcal{D}x \int \mathcal{D}\hat{x} \; J \exp\left[-i \int_0^t ds \; \hat{x}(s)\{E[x](s) - \xi(s)\}\right]$$

into the transition probability expression

- We have

$$
\begin{aligned}
&J(x_f, t|x_i, 0) \\
&= \int \mathcal{D}\xi \; P_\xi[\xi] \int_{x(0)=x_i}^{x(t)=x_f} \mathcal{D}x \int_{\hat{x}(0)=0}^{\hat{x}(t)=0} \mathcal{D}\hat{x} \; J \; \exp[-i \int_0^t ds \; \hat{x}(s)\{E[x](s) - \xi(s)\}] \\
&= \int_{x(0)=x_i}^{x(t)=x_f} \mathcal{D}x \int_{\hat{x}(0)=0}^{\hat{x}(t)=0} \mathcal{D}\hat{x} \; J \; \exp[-S_0[x, \hat{x}]],
\end{aligned}
$$

where

$$
\begin{aligned}
S_0[x, \hat{x}] \equiv \frac{1}{2} \int_0^t ds \int_0^t ds' \; \hat{x}(s)\Gamma(s - s')\hat{x}(s') \\
+ i \int_0^t ds \; \hat{x}(s)\Big\{m\ddot{x}(s) + \partial_x V(x, \lambda_s) + m \int_0^s ds' \; \gamma(s - s')\dot{x}(s')\Big\}
\end{aligned}
$$

- This is the same as the one obtained in the semiclassical expnasion (except for term from the initial preparation)

- The average of an observable $A[x(\tau)]$

$$\langle A[x(\tau)]\rangle = \int dx_f \int dx_i \; \rho_i(x_i) \int_{x(0)=x_i}^{x(t)=x_f} \mathcal{D}x \int \mathcal{D}\hat{x} \; J \; A[x(\tau)] e^{-S_0[x,\hat{x}]}$$
$$= \int \mathcal{D}x \int \mathcal{D}\hat{x} \; J \; A[x(\tau)] e^{-S_0[x,\hat{x}]} \rho_i(x_i),$$

where $\rho_i(x_i)$ is the initial distribution.

- Integrating out $\hat{x}$, we have the Onsager-Machlup action

$$\langle A[x(\tau)]\rangle \sim \int \mathcal{D}x \; A[x(\tau)] e^{-S_{OM}[x]} \rho_i(x_i),$$

where

$$S_{OM}[x] = \frac{1}{2} \int_0^t ds \int_0^t ds' \; E[x](s) G(s-s') E[x](s')$$

- $\mathcal{P}[x] \equiv \exp[-S_{OM}[x] + \ln \rho_i(x_i)]$ can be regarded as the probability for the path $x(s)$, $0 \le s \le t$

Classical Integral Fluctuation Theorem

- Conventionally Integral Fluctuation Theorem (IFT) for classical stochastic systems can be derived by considering the ratio between path probabilities

$$\mathcal{R}[x] = \ln \frac{\mathcal{P}[x]}{\mathcal{P}^{\mathrm{R}}[x^{\mathrm{R}}]}$$

  - $\mathcal{P}^{\mathrm{R}}[x^{\mathrm{R}}]$ for time-reversed path $x^{\mathrm{R}}(s) = x(t-s)$
  - $\mathcal{R} \to \Delta S_{\mathrm{tot}}$
  - IFT $\langle \exp(-\mathcal{R}[x]) \rangle = 1$, follows from the normalization of $\mathcal{P}^{\mathrm{R}}$.
  - $\langle \mathcal{R}[x] \rangle \geq 0$ from Jensen's inequality

- In quantum cases, integrating away x_q and obtaining $\mathcal{P}[x_c]$ are NOT straightforward

Time-reversal Transformations

- Consider the following transformation

$$\mathcal{R}: \begin{cases} x(s) & \rightarrow & x^{\mathrm{R}}(s) \equiv x(t-s) \\ \hat{x}(s) & \rightarrow & \hat{x}^{\mathrm{R}}(s) \equiv \hat{x}(t-s) - i\beta \frac{d}{ds} x(t-s) \end{cases}$$

- Integration measure:

$$\mathcal{D}x\mathcal{D}\hat{x} = \mathcal{D}x^{\mathrm{R}}\mathcal{D}\hat{x}^{\mathrm{R}}$$

- Note that $\Gamma(s-s') = \beta^{-1} m(\gamma(s-s') + \gamma(s'-s))$ where $\gamma(s-s')$ already contains $\Theta(s-s')$
- Calculate the change in S_0 under this transformation. First we rewrite

$$S_0[x,\hat{x}] = \int_0^t ds \int_0^t ds' \; \hat{x}(s) m\gamma(s-s') \left\{\beta^{-1}\hat{x}(s') + i\dot{x}(s')\right\} + i\int_0^t ds \; \hat{x}(s) \Big\{ m\ddot{x}(s) + \partial_x V(x,\lambda_s) \Big\}$$

$$
\begin{aligned}
S_0[x^{\mathrm{R}}, \hat{x}^{\mathrm{R}}; \lambda_s] &= \int_0^t ds \int_0^t ds' \{\hat{x}(t-s) - i\beta \frac{d}{ds} x(t-s)\} m\gamma(s-s') \\
&\qquad \times \{\beta^{-1}\hat{x}(t-s') - i\frac{d}{ds'}x(t-s') + i\frac{d}{ds'}x(t-s')\} \\
&\quad + i\int_0^t ds \, \{\hat{x}(t-s) - i\beta \frac{d}{ds}x(t-s)\} \\
&\qquad \times \left\{ m\frac{d^2}{ds^2}x(t-s) + \partial_x V(x(t-s), \lambda_s) \right\} \\
&= \int_0^t ds \int_0^t ds' \, \{\hat{x}(s) + i\beta \frac{d}{ds}x(s)\} m\gamma(s'-s)\beta^{-1}\hat{x}(s') \\
&\quad + i\int_0^t ds \, \{\hat{x}(s) + i\beta\frac{d}{ds}x(s)\}\left\{ m\frac{d^2}{ds^2}x(s) + \partial_x V(x(s), \lambda_{t-s})\right\} \\
&= S_0[x, \hat{x}; \lambda_{t-s}] \underbrace{-\beta \int_0^t ds \, \dot{x}(s)\{m\ddot{x}(s) + \partial_x V(x(s), \lambda_{t-s})\}}_{\equiv \Delta S_0[x, \lambda_{t-s}]}
\end{aligned}
$$

Symmetry of MSR functional at Equilibrium

- Consider the case where there is no explicit time dependence in $V(x)$. Then

$$\Delta S_0[x] = -\beta \int_0^t ds \, \frac{d}{ds}\{\frac{m}{2}\dot{x}^2(s) + V(x(s))\} = -\beta\{H(x(t)) - H(x(0))\}$$

- Consider the case where the initial and final distributions are given by

$$\rho(x) = \frac{1}{Z} e^{-\beta H(x)}$$

- We then have the symmetry

$$\begin{aligned} \langle \mathcal{O}[x, \hat{x}] \rangle &= \int \mathcal{D}x \int \mathcal{D}\hat{x} \, \mathcal{O}[x, \hat{x}] e^{-S_0[x,\hat{x}]} \rho(x(0)) \\ &= \int \mathcal{D}x^{\mathrm{R}} \int \mathcal{D}\hat{x}^{\mathrm{R}} \, \mathcal{O}[x^{\mathrm{R}}, \hat{x}^{\mathrm{R}}] e^{-S_0[x^{\mathrm{R}},\hat{x}^{\mathrm{R}}]} \rho(x^{\mathrm{R}}(0)) \\ &= \int \mathcal{D}x \int \mathcal{D}\hat{x} \, \mathcal{O}[x^{\mathrm{R}}, \hat{x}^{\mathrm{R}}] e^{-S_0[x,\hat{x}] + \beta\{H(x(t)) - H(x(0))\}} \rho(x(t)) \\ &= \int \mathcal{D}x \int \mathcal{D}\hat{x} \, \mathcal{O}[x^{\mathrm{R}}, \hat{x}^{\mathrm{R}}] e^{-S_0[x,\hat{x}]} \rho(x(0)) \\ &= \langle \mathcal{O}[x^{\mathrm{R}}, \hat{x}^{\mathrm{R}}] \rangle \end{aligned}$$

Time-reversal Transformations in Nonequilibrium

- In the presence of time-dep. protocol, $(\lambda^{\rm R}_s \equiv \lambda_{t-s})$

$$S_0[x^{\rm R}, \hat{x}^{\rm R}; \lambda] = S_0[x, \hat{x}; \lambda^{\rm R}] + \Delta S_0[x; \lambda^{\rm R}],$$

where

$$\Delta S_0[x; \lambda^{\rm R}] = -\beta \int_0^t ds\, \dot{x}(s)\{m\ddot{x}(s) + \partial_x V(x(s), \lambda_{t-s})\} = -\Delta S_0[x^{\rm R}; \lambda]$$

Now consider

$$
\begin{aligned}
& \left\langle \mathcal{O}[x,\hat{x}] e^{-\Delta S[x;\lambda] - \ln \rho_i(x(0)) + \ln \rho_f(x(t))} \right\rangle \\
= & \int \mathcal{D}x \int \mathcal{D}\hat{x}\, \mathcal{O}[x,\hat{x}] e^{-S_0[x,\hat{x};\lambda] - \Delta S_0[x;\lambda]} \frac{\rho_f(x(t))}{\rho_i(x(0))} \rho_i(x(0)) \\
= & \int \mathcal{D}x^{\mathrm{R}} \int \mathcal{D}\hat{x}^{\mathrm{R}}\, \mathcal{O}[x^{\mathrm{R}},\hat{x}^{\mathrm{R}}] e^{-S_0[x^{\mathrm{R}},\hat{x}^{\mathrm{R}};\lambda] - \Delta S_0[x^{\mathrm{R}};\lambda]} \rho_f(x^{\mathrm{R}}(t)) \\
= & \int \mathcal{D}x \int \mathcal{D}\hat{x}\, \mathcal{O}[x^{\mathrm{R}},\hat{x}^{\mathrm{R}}] e^{-S_0[x,\hat{x};\lambda^{\mathrm{R}}] - \Delta S_0[x;\lambda^{\mathrm{R}}] + \Delta S_0[x;\lambda^{\mathrm{R}}]} \rho_f(x(0)) \\
= & \int \mathcal{D}x \int \mathcal{D}\hat{x}\, \mathcal{O}[x^{\mathrm{R}},\hat{x}^{\mathrm{R}}] e^{-S_0[x,\hat{x};\lambda^{\mathrm{R}}]} \rho_f(x(0)) \\
\equiv & \left\langle \mathcal{O}[x^{\mathrm{R}},\hat{x}^{\mathrm{R}}] \right\rangle_{\mathrm{R}},
\end{aligned}
$$

where $\langle \cdots \rangle_{\mathrm{R}}$ is the average evaluated with the reverse protocol λ^{R} and the initial distribution ρ_f

- Note that one can rewrite

$$\Delta S_0[x;\lambda] = -\beta \int_0^t ds\ \dot{x}(s) \left[-m \int_0^s ds'\ \gamma(s-s')\dot{x}(s') + \xi(s) \right]$$

The quantity in $[\cdots]$ is the force from the reservoir and the integral can usually be interpreted as the heat flow ΔQ into the system. We therefore have

$$\Delta S_0[x;\lambda] = -\frac{\Delta Q}{T} = \Delta S_{\rm env}$$

which is the entropy change in the environment (reservoir).

- Let us write the system entropy change as the change in Shannon entropy as

$$\Delta S_{\rm sys} = -\ln \rho_f(x(t)) + \ln \rho_i(x(0))$$

- The total entropy change is $\Delta S_{\rm tot} = \Delta S_{\rm sys} + \Delta S_{\rm env}$

Integral Fluctuation Theorem

- The above relation can then be written as

$$\boxed{\left\langle \mathcal{O}[x,\hat{x}]e^{-\Delta S_{\rm tot}}\right\rangle = \left\langle \mathcal{O}[x^{\rm R},\hat{x}^{\rm R}]\right\rangle_{\rm R}}$$

- For $\mathcal{O} = 1$, we have the integral fluctuation theorem

$$\boxed{\left\langle e^{-\Delta S_{\rm tot}}\right\rangle = 1}.$$

From Jensen's inequality $\langle e^x\rangle \geq e^{\langle x\rangle}$, the thermodynamic 2nd law follows

$$\langle \Delta S_{\rm tot}\rangle \geq 0$$

Jarzynski equality

- We have

$$\Delta S_{\rm env} = -\beta \int_0^t ds\, \dot{x}(s)\{m\ddot{x}(s) + \partial_x V(x(s), \lambda_s)\}$$

$$= -\beta \int_0^t ds \left[\frac{dH}{ds} - \dot{\lambda}_s \frac{\partial V}{\partial \lambda_s}\right] = -\frac{\Delta H}{T} + \frac{\Delta W}{T},$$

where $\Delta H = H(x(t); \lambda_t) - H(x(0); \lambda_0)$ with

$$H(x(s); \lambda_s) = \frac{1}{2} m\dot{x}^2(s) + V(x(s), \lambda_s)$$

and the Jarzynski work

$$\Delta W = \int_0^t ds\, \dot{\lambda}_s \frac{\partial V}{\partial \lambda_s}$$

- Consider also the case where the initial and final distributions are given by Boltzmann distribution as

$$\rho_i(x(0)) = \frac{1}{Z(0)} e^{-\beta H(x(0);\lambda_0)}, \qquad \rho_f(x(t)) = \frac{1}{Z(t)} e^{-\beta H(x(t);\lambda_t)}$$

- The system entropy change is

$$\Delta S_{\rm sys} = -\ln \rho_f(x(t), \lambda_t) + \ln \rho_f(x(0), \lambda_0) = \frac{1}{T}(\Delta H - \Delta F),$$

  where $\Delta F = -T \ln Z(\tau) + T \ln Z(0)$ is the free energy difference.
- The total entropy change is

$$\Delta S_{\rm tot} = \Delta S_{\rm env} + \Delta S_{\rm sys} = \frac{\Delta W}{T} - \frac{\Delta F}{T}$$

- Applying this to the above identity, we have

$$e^{\Delta F/T} \left\langle \mathcal{O}[x, \hat{x}] e^{-\Delta W/T} \right\rangle = \langle \mathcal{O}[x^{\rm R}, \hat{x}^{\rm R}] \rangle_{\rm R0} ,$$

  where $\langle \cdots \rangle_{\rm R0}$ is the average using the reverse protocol and the Boltzmann distribution as an initial one.
- When $\mathcal{O} = 1$,

$$\boxed{\langle e^{-\Delta W/T} \rangle = e^{-\Delta F/T}} \quad \Rightarrow \langle \Delta W \rangle \geq \Delta F$$

Summary

- We have obtained a closed form for the time evolution of reduced density matrix for System (obtained by tracing out the Bath) for quantum Brownian motion
- The formalism is apparently without approximations (i.e. Markov, Ohmic bath, weak interaction etc.)
- The detailed form depends on the preparation of the initial state.
- The classical limit of corresponds to the MSR path integral expression for a generalized Langevin equation with a damping term with memory.
- Classically, equilibrium is characterized by the symmetry of MSR action under a time-reversal transformation.
- Classical Fluctuation Theorem (FT) can be obtained from the behavior of the MSR action under this time reversal transformation

Outlook

- Conventional method to obtain classical FT is to use the ratio between Onsager-Machlup path probabilities, $\exp[-S_{OM}[x]]$ for a path $x(s)$ and its time-reversed one $x^{\mathrm{R}}(s)$.
- In Quantum case, there is no corresponding quantity, since one cannot easily integrate away $x_q(s)$.
- One has to rely on the formalism that involves two fields, $x_c(s)$ and $x_q(s)$.
- First task is to find appropriate transformations

$$x_c(s) \to x_c^{\mathrm{R}}(s), \qquad x_q(s) \to x_q^{\mathrm{R}}(s)$$

  such that they leave the action invariant in equilibrium situation.
- Program: Equilibrium $\leftarrow$ symmetry of action under the transformation, Noneq. FT $\leftarrow$ breaking of symmetry