Local times in path integrals

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Outline

- **Some basics**
  - Quantum evolution $\leftrightarrow$ Thermal density matrix $\leftrightarrow$ Diffusion
  - Diffusion equation, Spectral representation
  - Feynman path integral, Local-time path integral
  - High-temperature ($\leftrightarrow$ short-time) expansion
- **Local-time path integral**
  - Local time: definition and basic properties
  - Low-temperature ($\leftrightarrow$ long-time) regime
  - Generic functionals of the local time
- **Summary and open questions**

Quantum evolution $\leftrightarrow$ Thermal density matrix $\leftrightarrow$ Diffusion

Quantum mechanics in 1D, time-independent:

$$\hat{H} = \frac{\hat{p}^2}{2M} + V(\hat{x}) \quad , \qquad \hat{p}|x\rangle = -i\hbar\frac{\partial}{\partial x}|x\rangle$$

- Quantum evolution operator: $e^{-it\hat{H}/\hbar}$

  $\downarrow$ Wick rotation ($t \to -i\hbar\beta$) $\downarrow$

- Gibbs operator: $e^{-\beta\hat{H}}$

  $\to$ partition function: $Tr(e^{-\beta\hat{H}}) \quad , \qquad \beta = 1/k_B T$

  $\to$ thermal density matrix: $e^{-\beta\hat{H}}/Tr(e^{-\beta\hat{H}})$

$$\rho(x_a, x_b, \beta) \equiv \langle x_b|e^{-\beta\hat{H}}|x_a\rangle$$

- ρ ... Heat kernel for diffusion generated by $\hat{H}$, with time variable β

Representations of $\rho(x_a, x_b, \beta)$

- Diffusion equation (without drift):

$$\frac{\partial \rho}{\partial \beta} = \left[\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x_b^2} - V(x_b)\right]\rho \quad \text{with} \quad \rho(x_a, x_b, 0_+) = \delta(x_b - x_a)$$

- Spectral representation:

$$\sum_n e^{-\beta E_n}\psi_n^*(x_a)\psi_n(x_b) \quad \text{where} \quad \hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$$

- Feynman path integral:

$$\int_{x(0)=x_a}^{x(\beta\hbar)=x_b} \mathcal{D}x(\tau)\exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{M}{2}\dot{x}^2(\tau) + V(x(\tau))\right]\right\}$$

- Local-time path integral: path integral over x-dependent paths

Feynman path integral

- $\beta \to 0$ ... short-time diffusion $\leftrightarrow$ high temperatures:

$$V(x(\tau)) = V(x_a) + V'(x_a)(x(\tau) - x_a) + \ldots \Rightarrow \rho \sim \frac{e^{-\beta V(x_a)}}{\sqrt{2\pi\beta\hbar^2/M}}$$

Path-integral approach to the Wigner-Kirkwood expansion
P. Jizba and V. Zatloukal, Phys. Rev. E **89**, 012135 (2014)

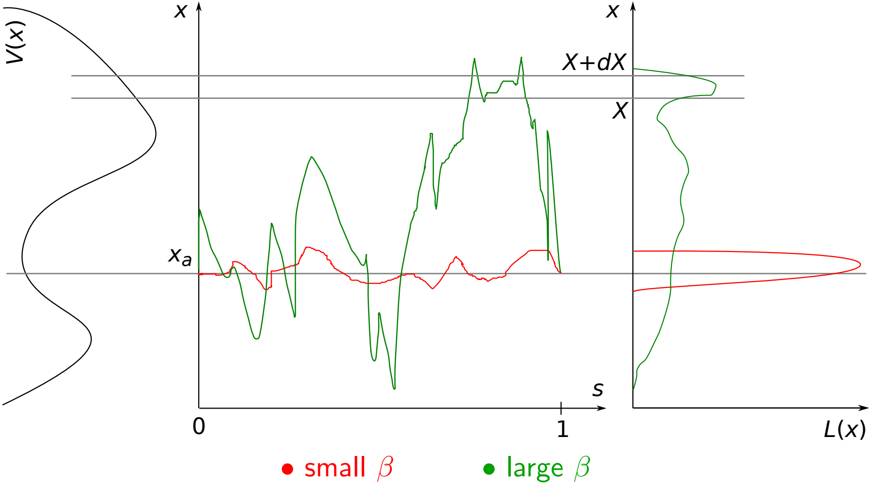
- $\beta \to \infty$ ... long-time diffusion $\leftrightarrow$ low temperatures:

$$\text{spectral representation} \quad \Rightarrow \quad \rho \sim e^{-\beta E_{gs}} \psi^*_{gs}(x_a) \psi_{gs}(x_b)$$

$\mathcal{Q}$: How to derive it from path integral?

Paths $x(\tau)$ vs. $L(x)$

$\tau \to s = \tau/\beta\hbar$



Local time: definition and basic properties

Rewriting the potential part of the action

$$\int_0^{\beta\hbar} d\tau V(x(\tau)) = \int_0^{\beta\hbar} d\tau \int_{\mathbb{R}} dX \delta(X - x(\tau)) V(X)$$

$$\Rightarrow \quad \textbf{Local time:} \quad L[x(\tau)](X) \equiv \int_0^{\beta\hbar} d\tau \delta(X - x(\tau))$$

Functional of $x(\tau)$, function of X:

- $L(X) \geq 0$
- $\int_{\mathbb{R}} L(X) dX = \beta\hbar$
- $L(X)$ has compact support
- $L(X)$ is continuous

Local-time path integral

For the full path integral we thus have

$$\rho(x_a, x_b, \beta) = \int_{x(0)=x_a}^{x(\beta\hbar)=x_b} \mathcal{D}x(\tau) \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} \frac{M}{2}\dot{x}^2(\tau)d\tau - \frac{1}{\hbar}\int_{\mathbb{R}} V(X)L(X)dX\right\}$$

$$\Downarrow$$

change of variables: $x(\tau) \ \rightarrow \ L(X)$

$$\Downarrow$$

$$\rho(x_a, x_b, \beta) = \int \mathcal{D}L(x) W[L(x); \beta\hbar, x_a, x_b] \exp\left\{-\int_{\mathbb{R}} L(x)V(x)dx\right\}$$

where $L(x) \geq 0$ and $W[L(x)] = 0$ if $\int_{\mathbb{R}} L(x)dx \neq \beta\hbar$

Local-time path integral: glimpses of the derivation

- Diffusion equation in Laplace picture:
  $\left[E - \frac{\hbar^2}{2M}\frac{\partial^2}{\partial x_b^2} + V(x_b)\right]\widetilde{\rho}(x_a, x_b, E) = \delta(x_a - x_b)$

- Quantum-field-theoretic representation:
  $\widetilde{\rho}(x_a, x_b, E) = 2\int \mathcal{D}\psi(x)\psi(x_a)\psi(x_b)e^{-\langle\psi|E+\hat{H}|\psi\rangle} / \int \mathcal{D}\psi(x)e^{-\langle\psi|E+\hat{H}|\psi\rangle}$

- Replica trick: $a/b = \lim_{D\to 0} ab^{D-1}$

  $\widetilde{\rho} = \lim_{D\to 0}\frac{2}{D}\int \mathcal{D}^D\psi(x)\psi_1(x_a)\psi_1(x_b)\exp\left\{-\sum_{\sigma=1}^{D}\langle\psi_\sigma|E+\hat{H}|\psi_\sigma\rangle\right\}$

- Spherical coordinates in ψ-space: radial part $\eta = \sqrt{\vec{\psi}\cdot\vec{\psi}}$

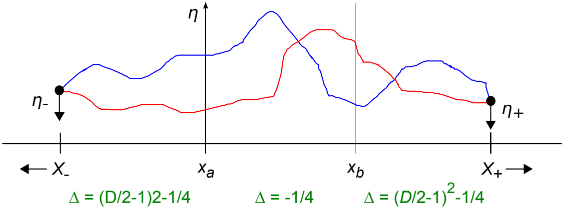
- Inverse Laplace transform $\Rightarrow$ *Local-time representation of* $\rho(x_a, x_b, \beta)$

Local-time path integral

Local-time representation:

$$\rho(x_a, x_b, \beta) \equiv \langle x_b | e^{-\beta \hat{H}} | x_a \rangle = \lim_{X_\pm \to \pm\infty} \lim_{D \to 0} \frac{2}{D^2} \lim_{\eta_\pm \to 0} (\eta_- \eta_+)^{\frac{1-D}{2}}$$

$$\times \int_{\eta(X_-)=\eta_-}^{\eta(X_+)=\eta_+} \mathcal{D}\eta(x) \delta\left(\int_{X_-}^{X_+} \eta^2(x) dx - \beta \right) \eta(x_a) \eta(x_b) \exp\left\{ -A_\Delta[\eta(x)] \right\}$$



where

- $\eta(x) \geq 0$, $\eta^2(x) \leftrightarrow L(x)/\hbar$
- $A_\Delta[\eta(x)] \equiv \int_{X_-}^{X_+} dx \left[\frac{\hbar^2}{2M} \eta'(x)^2 + V(x)\eta^2(x) + \frac{M}{\hbar^2} \frac{\Delta(x)}{2\eta^2(x)} \right]$
  - Action of the radial harmonic oscillator ($\leftrightarrow$ Bessel process)
  - Time variable x, Radial coordinate η

Local-time path integral at $\beta \to \infty$

Rescaling $\eta \to \sqrt{\beta}\eta$:

$$A_\Delta[\sqrt{\beta}\eta(x)] = \beta \int_{X_-}^{X_+} dx \left[\frac{\hbar^2}{2M}\eta'(x)^2 + V(x)\eta^2(x) + \frac{M}{\hbar^2}\frac{\Delta(x)}{2\beta^2\eta^2(x)} \right]$$

Saddle-point approximation of the path integral (neglecting the last term)
$\leftrightarrow$ Minimization of the functional:

$$\int_{X_-}^{X_+} dx \left[\frac{\hbar^2}{2M}\eta'(x)^2 + V(x)\eta^2(x) \right] = \langle \eta | \hat{H} | \eta \rangle$$

under the constraint: $\delta\left(\int_{X_-}^{X_+} \eta^2(x)dx - 1 \right) \leftrightarrow \langle \eta | \eta \rangle = 1$

$\Rightarrow$ Rayleigh-Ritz variational principle for the ground state

Generic functionals of the local time

Average value of arbitrary functional F:

$$\bar{F}(x_a, x_b, \beta) \equiv \int_{x(0)=x_a}^{x(\beta\hbar)=x_b} \mathcal{D}x(\tau) F[L(X)] \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\frac{M}{2}\dot{x}^2(\tau) + V(x(\tau))\right]\right\}$$

F is a functional of $L(X) = \int_0^{\beta\hbar} d\tau \delta(X - x(\tau))$

(E.g.: $F[L(X)] = L(0) \to \bar{F}$ ... average time spent at the origin)

Since $\int_0^{\beta\hbar} d\tau V(x(\tau)) = \int_{\mathbb{R}} dX \; L(X) V(X)$, $\quad F[L(X)] \;\leftrightarrow\; F\left[\frac{-\hbar\delta}{\delta V(X)}\right]$

$$\Rightarrow \quad \bar{F}(x_a, x_b, \beta) = F\left[\frac{-\hbar\delta}{\delta V(X)}\right] \rho(x_a, x_b, \beta)$$

Generic functionals of the local time

Our most general result:

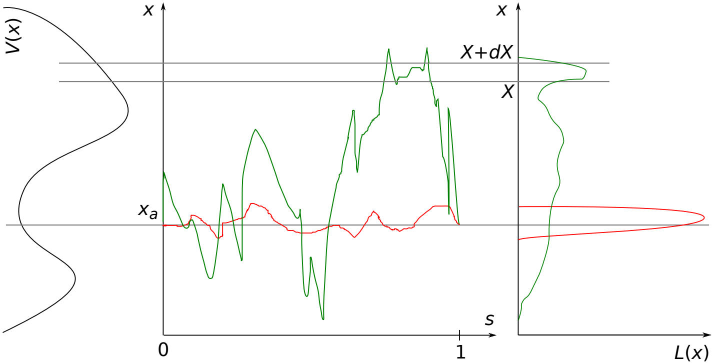
$$\bar{F}(x_a, x_b, \beta) = \lim_{X_\pm \to \pm\infty} \lim_{D\to 0} \frac{2}{D^2} \lim_{\eta_\pm \to 0} (\eta_- \eta_+)^{\frac{1-D}{2}}$$

$$\times \int_{\eta(X_-)=\eta_-}^{\eta(X_+)=\eta_+} \mathcal{D}\eta(x) F[\hbar\eta^2(x)] \delta\left(\int_{X_-}^{X_+} \eta^2(x) dx - \beta\right) \eta(x_a)\eta(x_b) e^{-A_\Delta[\eta(x)]}$$

Choice of F relevant for applications in stochastic processes, statistical physics, etc. is an open issue → suggestions are welcomed!

Summary

- Diffusion equation → Feynman path integral
- ↪ Local-time path-integral representation of $\langle x_b | e^{-\beta \hat{H}} | x_a \rangle$
- Including arbitrary functionals of the local time



Open questions

- $\mathcal{Q}$: Rigorous derivations of the $\beta \to \infty$-limit and first corrections.
- $\mathcal{Q}$: Physical applications of the formula for arbitrary functionals.

- $\mathcal{Q}$: What about higher-dimensional quantum mechanics ($x \in \mathbb{R}^n$)?
- $\mathcal{Q}$: What about quantum field theory ($\tau \in \mathbb{R}^d$)?

Details in: V. Zatloukal and P. Jizba, *in preparation*