Path integrals at high and low temperatures: Wigner-Kirkwood expansion and local-time representation

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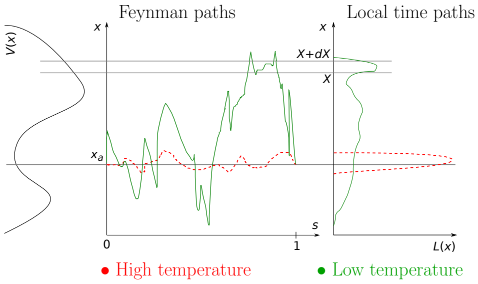
Introduction: Quantum statistical mechanics

Quantum-mechanical Hamiltonian: $\hat{H} = \sum_{j=1}^{D} \frac{\hat{p}_j}{2M_j} + V(\hat{\mathbf{x}})$

Gibbs operator: $e^{-\beta\hat{H}}$ $(\beta = 1/k_B T)$ $\rightarrow$ Partition function: $Z(\beta) = \mathrm{Tr} e^{-\beta\hat{H}}$

Feynman-Kac formula: $\langle \mathbf{x}_b | e^{-\beta\hat{H}} | \mathbf{x}_a \rangle = \int_{\mathbf{x}(0)=\mathbf{x}_a}^{\mathbf{x}(\beta\hbar)=\mathbf{x}_b} \mathcal{D}\mathbf{x}(\tau) \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left[\sum_{j=1}^{D} \frac{M_j}{2}\dot{x}_j^2 + V(\mathbf{x})\right]\right\}$



High temperatures: Wigner-Kirkwood expansion

High temperature $\leftrightarrow$ small β

Fluctuation controlled by λ_j and β.

Rescaled PI representation: $\mathbf{x}_b = \mathbf{x}_a$, $\mathbf{x} \rightarrow \mathbf{x}_a + \Lambda\boldsymbol{\xi}$, $\tau \rightarrow \beta\hbar s$:

$$\langle \mathbf{x}_a | e^{-\beta\hat{H}} | \mathbf{x}_a \rangle = \frac{1}{\det\Lambda} \int_{\boldsymbol{\xi}(0)=\mathbf{0}}^{\boldsymbol{\xi}(1)=\mathbf{0}} \mathcal{D}\boldsymbol{\xi}(s) \exp\left\{-\int_0^1 ds \left[\frac{1}{2}\dot{\boldsymbol{\xi}}^2 + \beta V(\mathbf{x}_a + \Lambda\boldsymbol{\xi})\right]\right\} \quad (1)$$

$(\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_D)$, $\lambda_j \equiv \sqrt{\beta\hbar^2/M_j}$ ... thermal wavelength)

Expand the potential term:

$$V(\mathbf{x}_a + \Lambda\boldsymbol{\xi}(s)) = V(\mathbf{x}_a) + \sum_{\mathbf{m}\neq\mathbf{0}} \frac{V^{(\mathbf{m})}(\mathbf{x}_a)}{\mathbf{m}!}(\Lambda\boldsymbol{\xi}(s))^{\mathbf{m}} \quad (2)$$

$\Rightarrow$ Wigner-Kirkwood expansion:

$$\langle \mathbf{x}_a | e^{-\beta\hat{H}} | \mathbf{x}_a \rangle = \frac{e^{-\beta V(\mathbf{x}_a)}}{\det\Lambda} \sum_{n=0}^{\infty} (-\beta)^n \sum_{\mathbf{m}_1,\ldots,\mathbf{m}_n\neq\mathbf{0}} \prod_{j=1}^{D} \lambda_j^{m_1^j+\ldots+m_n^j} \frac{V^{(\mathbf{m}_1)}(\mathbf{x}_a)\ldots V^{(\mathbf{m}_n)}(\mathbf{x}_a)}{\mathbf{m}_1!\ldots\mathbf{m}_n!} Q \quad (3)$$

with the coefficients $Q(\mathbf{m}_1, \ldots, \mathbf{m}_n)$ given by

$$Q = \int_{0<s_1<\ldots<s_n<1} ds_1 \ldots ds_n \int_{\boldsymbol{\xi}(0)=\mathbf{0}}^{\boldsymbol{\xi}(1)=\mathbf{0}} \mathcal{D}\boldsymbol{\xi}(s) \boldsymbol{\xi}^{\boldsymbol{m}_1}(s_1)\ldots\boldsymbol{\xi}^{\boldsymbol{m}_n}(s_n) \exp\left[-\int_0^1 ds \frac{1}{2}\dot{\boldsymbol{\xi}}^2(s)\right]$$
$$= K \int_{\mathbb{R}^D} \frac{d\mathbf{q}}{(2\pi)^D} \left(\frac{i^{|\mathbf{m}_n|}}{1+\frac{\mathbf{q}^2}{2}} \frac{\partial^{|\mathbf{m}_n|}}{\partial\mathbf{q}^{\mathbf{m}_n}}\right) \ldots \left(\frac{i^{|\mathbf{m}_1|}}{1+\frac{\mathbf{q}^2}{2}} \frac{\partial^{|\mathbf{m}_1|}}{\partial\mathbf{q}^{\mathbf{m}_1}}\right) \frac{1}{1+\frac{\mathbf{q}^2}{2}} \quad (4)$$

where the multiplicative constant has the form: $1/K = \Gamma\left(n + 1 - \frac{D}{2} + \frac{|\boldsymbol{m}_1|+\ldots+|\boldsymbol{m}_n|}{2}\right)$

WK expansion of the off-diagonal matrix elements $\langle \mathbf{x}_b | e^{-\beta\hat{H}} | \mathbf{x}_a \rangle$ with a help of the world-line Green functions of Onofri and Zuk.

One-dimensional system

$$Q = \frac{\left(\frac{m_1+\ldots+m_n}{2} + n\right)!}{\sqrt{2\pi}\, 2^{(m_1+\ldots+m_n)/2}} \sum_{\ell_1=0}^{m_1} \cdots \sum_{\ell_n=0}^{m_n} \prod_{k=1}^{n} \frac{(-1)^{\ell_k}\binom{m_k}{\ell_k}}{(\ell_1+\ldots+\ell_k+k)(m_1-\ell_1+\ldots+m_k-\ell_k+k)} \quad (5)$$

Coefficients of the series $e^{\beta V(x)}\sqrt{2\pi}\lambda \langle x | e^{-\beta\hat{H}} | x \rangle$ at terms $\beta^i(\hbar^2)^j$:

	$\hbar^0$	$\hbar^2$	$\hbar^4$	$\hbar^6$	$\hbar^8$
β^0	1	0	0	0	0
β^1	0	0	0	0	0
β^2	0	$-\frac{V''(x)}{12M}$	0	0	0
β^3	0	$\frac{V'(x)^2}{24M}$	$-\frac{V^{(4)}(x)}{240M^2}$	0	0
β^4	0	0	$\frac{V''(x)^2}{160M^2} + \frac{V'(x)V^{(3)}(x)}{120M^2}$	$-\frac{V^{(6)}(x)}{6720M^3}$	0
β^5	0	0	$-\frac{11V'(x)^2V''(x)}{1440M^2}$	$\frac{23V^{(3)}(x)^2}{40320M^3} + \frac{19V''(x)V^{(4)}(x)}{20160M^3} + \frac{V'(x)V^{(5)}(x)}{2240M^3}$	$-\frac{V^{(8)}(x)}{241920M^4}$

Up to β^{18} with Wolfram Mathematica.

P. Jizba and V. Zatloukal, *Path-integral approach to the Wigner-Kirkwood expansion*, Phys. Rev. E **89**, 012135 (2014) [arXiv:1309.0206]

Low temperatures: Local-time path integral

Local time quantifies the time that the sample paths in the Feynman PI spend in the vicinity of an arbitrary point X (assume $D = 1$):

$$L(X) \equiv \int_0^{\beta\hbar} d\tau\, \delta(X - x(\tau)) \quad (6)$$

Change of stochastic variables: $x(\tau)$ (Feynman PI) $\Rightarrow$ $L(x)$ (Local-time PI)

Start from the field-theoretic PI representation of the resolvent:

$$\langle x_b | \frac{1}{\hat{H}+E} | x_a \rangle = \frac{\int \mathcal{D}\psi(x)\psi(x_a)\psi(x_b) e^{-\frac{1}{2}\langle\psi|E+\hat{H}|\psi\rangle}}{\int \mathcal{D}\psi(x) e^{-\frac{1}{2}\langle\psi|E+\hat{H}|\psi\rangle}} \quad (7)$$

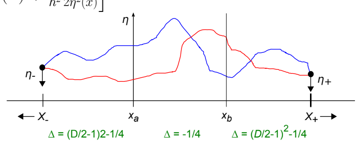
Replica trick ($\eta \geq 0$ ... radial field component)

$\Rightarrow$ Local-time path-integral representation

$$\langle x_b | e^{-\beta\hat{H}} | x_a \rangle = \lim_{X_\pm\rightarrow\pm\infty} \lim_{D\rightarrow 0} \frac{2}{D^2} \lim_{\eta_\pm\rightarrow 0} (\eta_-\eta_+)^{\frac{1-D}{2}}$$
$$\int_{\eta(X_-)=\eta_-}^{\eta(X_+)=\eta_+} \mathcal{D}\eta(x)\, \delta\left(\int_{X_-}^{X_+} \eta^2(x)dx - \beta\right) \eta(x_a)\eta(x_b) \exp\{-A_\Delta[\eta(x)]\} \quad (8)$$

Action of a radial harmonic oscillator with frequency $V(x)$:
$A_\Delta[\eta(x)] \equiv \int_{X_-}^{X_+} dx \left[\frac{\hbar^2}{2M}\eta'(x)^2 + V(x)\eta^2(x) + \frac{M}{\hbar^2}\frac{\Delta(x)}{2\eta^2(x)}\right]$

We identify $L(x) = \hbar\eta^2(x)$, where η follows the Bessel stochastic process.



The obtained relationship between the local-time representation of PI and the radial PI provides a practical illustration of the Ray-Knight theorem of the stochastic calculus.

Saddle-point approximation

Rescaling $\eta \rightarrow \sqrt{\beta}\eta$, $\beta \rightarrow \infty \Rightarrow$ Minimize functional $\langle\eta|\hat{H}|\eta\rangle$ for $\langle\eta|\eta\rangle = 1$

$\Updownarrow$

Rayleigh-Ritz variational principle for the ground state

P. Jizba and V. Zatloukal, *Local-time representation of path integrals*, (2015) [arXiv:1309.0206]

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