Fast Converging Path Integrals for Time-Dependent Potentials*

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*Supported by the Serbian-German bilateral research project PI-BEC, Serbian Ministry of Science research project No. OI141035, and EU CX-CMCS Centre of Excellence grant.

Overview

- Introduction
  - Path integral formalism
  - Discretized effective actions
  - Results for time-independent potentials
- Recursive approach
  - Schrödinger's equation
  - Recursive relations
- Numerical results
  - Forced harmonic oscillator
  - Time-dependent harmonic oscillator
  - Time-dependent pure quartic oscilator
- Conclusions and outlook

Path integral formalism (1)

- Amplitudes for transition from an initial state $|\mathbf{a}, t_a\rangle$ to a final state $|\mathbf{b}, t_b\rangle$ in imaginary time $T = t_b - t_a$:

$$A(\mathbf{a}, t_a; \mathbf{b}, t_b) = \langle \mathbf{b}, t_b | \hat{T} \exp\left\{ -\int_{t_a}^{t_b} dt\, \hat{H}(\hat{\mathbf{p}}, \hat{\mathbf{q}}, t) \right\} |\mathbf{a}, t_a\rangle$$

- Dividing the evolution into N time steps $\epsilon = T/N$, we get

$$A(\mathbf{a}, t_a; \mathbf{b}, t_b) = \int dq_1 \cdots dq_{N-1} A(\alpha, q_1; \epsilon) \cdots A(q_{N-1}, \beta; \epsilon)\,,$$

- Approximate calculation of short-time amplitudes leads to

$$A(\mathbf{a}, t_a; \mathbf{b}, t_b) = \frac{1}{(2\pi\epsilon)^{MdN/2}} \int dq_1 \cdots dq_{N-1}\, e^{-S_N}$$

- Hagen Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 5^{th} edition, World Scientific, Singapore, 2009.

Path integral formalism (2)

- Continual amplitude $A(\mathbf{a}, t_a; \mathbf{b}, t_b)$ is obtained in the limit $N \to \infty$ of the discretized amplitude $A_N(\mathbf{a}, t_a; \mathbf{b}, t_b)$,

$$A(\mathbf{a}, t_a; \mathbf{b}, t_b) = \lim_{N \to \infty} A_N(\mathbf{a}, t_a; \mathbf{b}, t_b)$$

- Discretized amplitude A_N is expressed as a multiple integral of the function e^{-S_N}, where S_N is called discretized action
- For a theory defined by the Hamiltonian operator $H(\mathbf{p}, \mathbf{q}, t) = \frac{1}{2}\,\mathbf{p}^2 + V(\mathbf{q}, t)$, (naive) discretized action is

$$S_N = \sum_{n=0}^{N-1} \left(\frac{\boldsymbol{\delta}_n^2}{2\epsilon} + \epsilon V(\mathbf{x}_n, \tau_n) \right) ,$$

where $\boldsymbol{\delta}_n = \mathbf{q}_{n+1} - \mathbf{q}_n$, $\mathbf{x}_n = \frac{\mathbf{q}_{n+1} + \mathbf{q}_n}{2}$, $\tau_n = \frac{t_n + t_{n+1}}{2}$.

Discretized effective actions

- Discretized actions can be classified according to the speed of convergence of discretized path integrals
- Improved discretized actions have been earlier constructed, mainly tailored for calculation of partition functions
  - split-operator techniques
  - multi-product expansion
- Sixth order expansion: Goldstein and Baye, PRE **70**, 056703 (2004)
- This cannot be easily extended to higher orders, nor such an approach was developed for general transition amplitudes
- We introduce the ideal short-time discretized action

$$S^*(\mathbf{x}, \boldsymbol{\delta}; \varepsilon, \tau) = \frac{\boldsymbol{\delta}^2}{2\varepsilon} + \varepsilon W(\mathbf{x}, \boldsymbol{\delta}; \varepsilon, \tau)$$

Results for time-independent potentials

- For time-independent potentials, we have developed a recursive formalism that allows calculation of the short-time expansion for W to arbitrary order in the time of propagation ε [PRE **79**, 036701 (2009)]
- Applied for accurate calculation of energy eigenstates and eigenvalues using the numerical diagonalization of the space-discretized matrix of the evolution operator [PRE **80**, 066705 (2009), PRE **80**, 066706 (2009)]
- One-time-step approximation to the path integral applied to the numerical study of properties of fast-rotating Bose-Einstein condensates, using the (very) high order effective potential [PLA **374**, 1539 (2010)]

Schrödinger's equation (1)

- We start from Schrödinger's equation for the short-time amplitude $A(\mathbf{a}, t_a; \mathbf{b}, t_b)$

$$\left[\partial_\varepsilon + \frac{1}{2}(\hat{H}_a + \hat{H}_b)\right] A(\mathbf{a}, t_a; \mathbf{b}, t_b) = 0\,,$$
$$\left[\partial_\tau + (\hat{H}_b - \hat{H}_a)\right] A(\mathbf{a}, t_a; \mathbf{b}, t_b) = 0\,,$$

where $\hat{H}_a = H(-i\boldsymbol{\partial}_\mathbf{a}, \mathbf{a}, t_a)$, $\varepsilon = t_b - t_a$, $\tau = (t_a + tb)/2$

- If we change the variables $\mathbf{a}$, $\mathbf{b}$ to $\mathbf{x}$ and $\bar{\mathbf{x}} = \boldsymbol{\delta}/2$, and write the amplitude as

$$A(\mathbf{x}, \bar{\mathbf{x}}; \varepsilon, \tau) = \frac{1}{(2\pi\varepsilon)^{Md/2}} e^{-\frac{2}{\varepsilon}\bar{\mathbf{x}}^2 - \varepsilon W(\mathbf{x}, \bar{\mathbf{x}}; \varepsilon, \tau)}\,,$$

we can obtain the equation for the effective potential W.

Schrödinger's equation (2)

- The equation for W:

$$W + \bar{\mathbf{x}} \cdot \bar{\boldsymbol{\partial}}\, W + \varepsilon \partial_\varepsilon W - \frac{1}{8}\, \varepsilon \partial^2 W - \frac{1}{8}\, \varepsilon \bar{\partial}^2 W + \frac{1}{8}\, \varepsilon^2 (\boldsymbol{\partial} W)^2 + \frac{1}{8}\, \varepsilon^2 (\bar{\boldsymbol{\partial}} W)^2 = \frac{1}{2}\, (V_+ + V_-)\,.$$

  where $V_\pm = V(\mathbf{x} \pm \bar{\mathbf{x}}, \tau \pm \varepsilon/2)$
- In order to solve it, we use short-time expansion of W in a form of double power series

$$W(\mathbf{x}, \bar{\mathbf{x}}; \varepsilon, \tau) = \sum_{m=0}^{\infty} \sum_{k=0}^{m} \left\{ W_{m,k}(\mathbf{x}, \bar{\mathbf{x}}; \tau)\, \varepsilon^{m-k} + W_{m+1/2,k}(\mathbf{x}, \bar{\mathbf{x}}; \tau)\, \varepsilon^{m-k} \right\},$$

$$W_{m,k}(\mathbf{x}, \bar{\mathbf{x}}; \tau) = \bar{x}_{i_1} \cdots \bar{x}_{i_{2k}}\, c_{m,k}^{i_1,\ldots i_{2k}}(\mathbf{x}; \tau)\,,$$

$$W_{m+1/2,k}(\mathbf{x}, \bar{\mathbf{x}}; \tau) = \bar{x}_{i_1} \cdots \bar{x}_{i_{2k+1}}\, c_{m+1/2,k}^{i_1,\ldots i_{2k+1}}(\mathbf{x}; \tau)\,,$$

Recursive relations (1)

- After inserting the expansion, we obtain two recursion relations for W coefficients:

$$8(m+k+1)\,W_{m,k} = 8\frac{\Pi(m,k)\,(\bar{\mathbf{x}}\cdot\boldsymbol{\partial})^{2k}\overset{(m-k)}{V}}{(2k)!\,(m-k)!\,2^{m-k}} + \bar{\partial}^2\,W_{m,k+1} + \partial^2\,W_{m-1,k}$$

$$-\sum_{l,r}\Big\{\boldsymbol{\partial}W_{l,r}\cdot\boldsymbol{\partial}W_{m-l-2,k-r} + \boldsymbol{\partial}W_{l+1/2,r}\cdot\boldsymbol{\partial}W_{m-l-5/2,k-r-1}$$

$$+\bar{\boldsymbol{\partial}}W_{l,r}\cdot\bar{\boldsymbol{\partial}}W_{m-l-1,k-r+1} + \bar{\boldsymbol{\partial}}W_{l+1/2,r}\cdot\bar{\boldsymbol{\partial}}W_{m-l-3/2,k-r}\Big\},$$

$$8(m+k+2)\,W_{m+1/2,k} = 8\frac{(1-\Pi(m,k))\,(\bar{\mathbf{x}}\cdot\boldsymbol{\partial})^{2k+1}\overset{(m-k)}{V}}{(2k+1)!\,(m-k)!\,2^{m-k}} + \bar{\partial}^2\,W_{m+1/2,k+1}$$

$$+\partial^2\,W_{m-1/2,k} - \sum_{l,r}\Big\{\boldsymbol{\partial}W_{l,r}\cdot\boldsymbol{\partial}W_{m-l-3/2,k-r} + \boldsymbol{\partial}W_{l+1/2,r}\cdot\boldsymbol{\partial}W_{m-l-2,k-r}$$

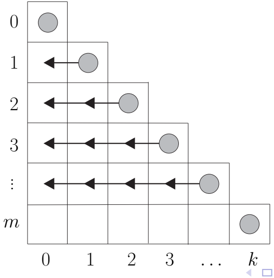
$$+\bar{\boldsymbol{\partial}}W_{l+1/2,r}\cdot\bar{\boldsymbol{\partial}}W_{m-l-1,k-r+1} + \bar{\boldsymbol{\partial}}W_{l,r}\cdot\bar{\boldsymbol{\partial}}W_{m-l-1/2,k-r+1}\Big\}.$$

Recursive relations (2)

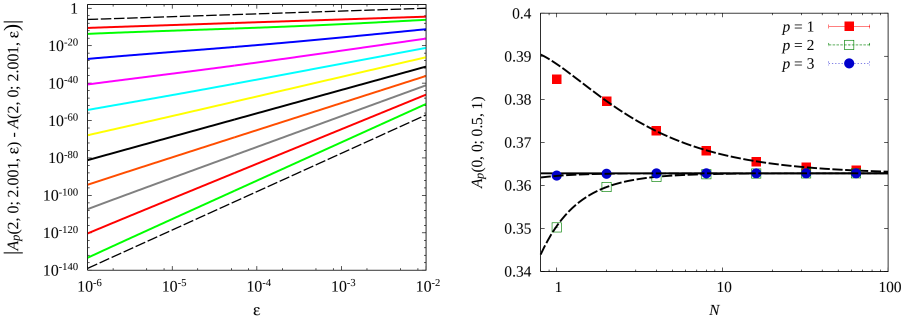
- Diagonal coefficients can be directly calculated

$$W_{m,m} = \frac{1}{(2m+1)!}(\bar{\mathbf{x}} \cdot \boldsymbol{\partial})^{2m} V \,,$$
$$W_{m+1/2,m} = 0 \,.$$

- Off-diagonal coefficients are obtained from recursions using the scheme

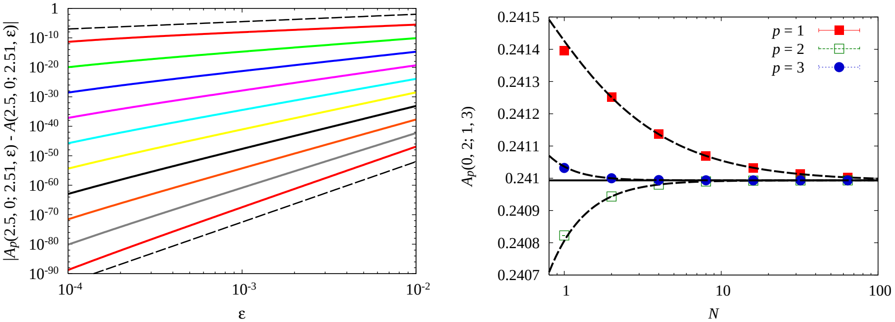


Forced harmonic oscillator



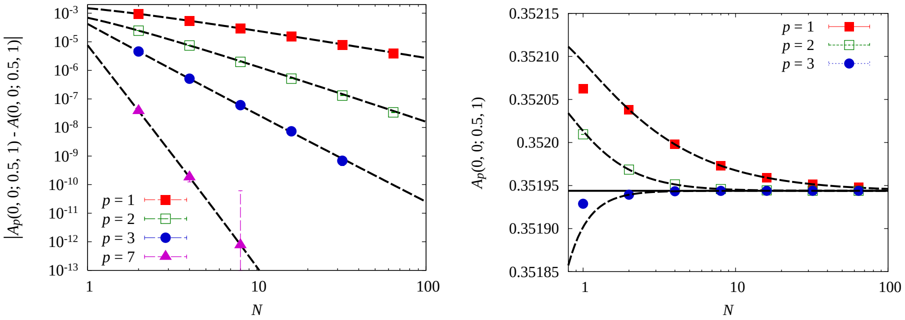
Convergence of discretized amplitudes for the forced harmonic oscillator $V_{\mathrm{FHO}}(x,t) = \frac{1}{2}\omega^2 x^2 - x \sin \Omega t$, with $\omega = \Omega = 1$ and $p = 1, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20$ from top to bottom on the left, and for long time of propagation using MC simulation with $N_{\mathrm{MC}} = 2 \cdot 10^9$ on the right.

Time-dependent harmonic oscillator



Convergence of discretized amplitudes for the time-dependent harmonic oscillator $V_{\mathrm{G,HO}}(x,t) = \frac{\omega^2 x^2}{2(1+t^2)^2}$, with $\omega = 1$ and $p = 2, 4, 6, 8, 10, 12, 14, 16, 18, 20$ from top to bottom on the left, and for long time of propagation using MC simulation with $N_{\mathrm{MC}} = 2 \cdot 10^9$ on the right.

Time-dependent pure quartic oscillator



Convergence of discretized amplitudes for the time-dependent pure quartic oscillator $V_{\mathrm{G,PQ}}(x,t) = \frac{gx^4}{24(1+t^2)^3}$, with $g = 0.1$ and $p = 1, 2, 3, 7$ from top to bottom on the left, and for long time of propagation using MC simulation with $N_{\mathrm{MC}} = 1.6 \cdot 10^{13}$ on the right.

Conclusions and outlook

- New method for analytic and numerical calculation of path integrals for a general time-dependent non-relativistic many-body quantum theory
- In the numerical approach, discretized effective actions of level p provide substantial speedup of Monte Carlo algorithm from $1/N$ to $1/N^p$
- If the time of propagation/inverse temperature is small, analytic one-time-step approximation can be used: path integrals without integrals
- We plan to use this approach to study quantum dynamics
    - Evolution in real and imaginary time
    - Solving of Gross-Pitaevskii-type equations
- AB, I. Vidanović, A. Bogojević, A. Pelster, arXiv:0912.2743