



Fast Converging Path Integrals for Time-Dependent Potentials*

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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*, 5th 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 $N \rightarrow \infty$ of the discretized amplitude $A_N(\mathbf{a}, t_a; \mathbf{b}, t_b)$,

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

- 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

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

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



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 $\hat{H}_a = H(-i\partial_{\mathbf{a}}, \mathbf{a}, t_a)$, $\varepsilon = t_b - t_a$, $\tau = (t_a + t_b)/2$

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

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

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

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

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

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



Recursive relations (1)

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

$$\begin{aligned}
 8(m+k+1)W_{m,k} &= 8 \frac{\Pi(m,k) (\bar{\mathbf{x}} \cdot \boldsymbol{\partial})^{2k} V^{(m-k)}}{(2k)! (m-k)! 2^{m-k}} + \bar{\partial}^2 W_{m,k+1} + \partial^2 W_{m-1,k} \\
 &\quad - \sum_{l,r} \left\{ \partial W_{l,r} \cdot \partial W_{m-l-2,k-r} + \partial W_{l+1/2,r} \cdot \partial W_{m-l-5/2,k-r-1} \right. \\
 &\quad \left. + \bar{\partial} W_{l,r} \cdot \bar{\partial} W_{m-l-1,k-r+1} + \bar{\partial} W_{l+1/2,r} \cdot \bar{\partial} W_{m-l-3/2,k-r} \right\}, \\
 8(m+k+2)W_{m+1/2,k} &= 8 \frac{(1-\Pi(m,k)) (\bar{\mathbf{x}} \cdot \boldsymbol{\partial})^{2k+1} V^{(m-k)}}{(2k+1)! (m-k)! 2^{m-k}} + \bar{\partial}^2 W_{m+1/2,k+1} \\
 &\quad + \partial^2 W_{m-1/2,k} - \sum_{l,r} \left\{ \partial W_{l,r} \cdot \partial W_{m-l-3/2,k-r} + \partial W_{l+1/2,r} \cdot \partial W_{m-l-2,k-r} \right. \\
 &\quad \left. + \bar{\partial} W_{l+1/2,r} \cdot \bar{\partial} W_{m-l-1,k-r+1} + \bar{\partial} W_{l,r} \cdot \bar{\partial} W_{m-l-1/2,k-r+1} \right\}.
 \end{aligned}$$



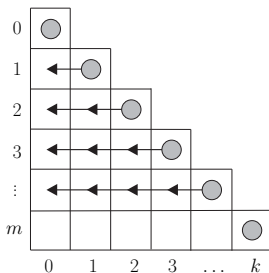
Recursive relations (2)

- Diagonal coefficients can be directly calculated

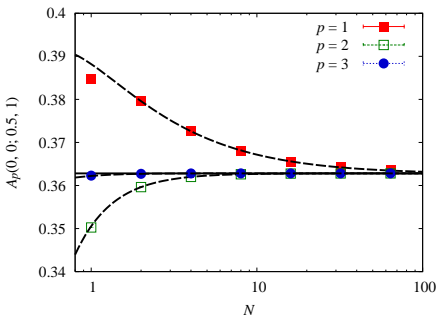
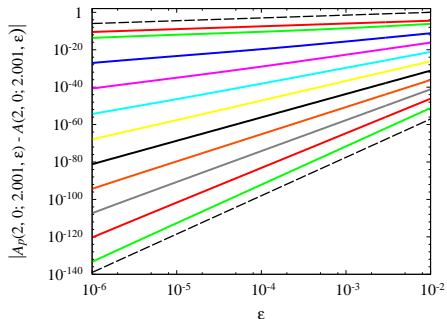
$$W_{m,m} = \frac{1}{(2m+1)!} (\bar{\mathbf{x}} \cdot \boldsymbol{\partial})^{2m} V,$$

$$W_{m+1/2,m} = 0.$$

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

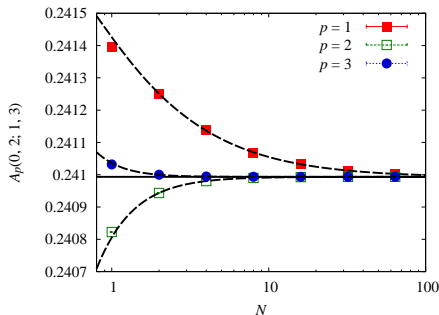
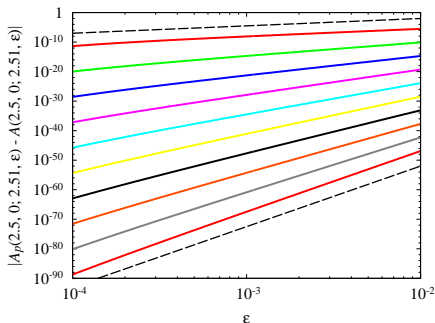


Forced harmonic oscillator



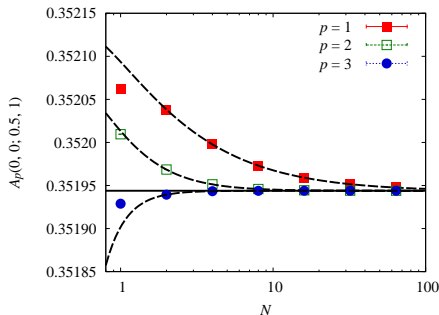
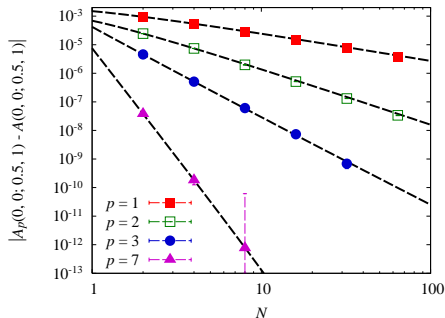
Convergence of discretized amplitudes for the forced harmonic oscillator $V_{\text{FHO}}(x, t) = \frac{1}{2}\omega^2 x^2 - x \sin \Omega t$, with $\omega = \Omega = 1$ and $p = 1, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20$ (left, top to bottom), and for long time of propagation using MC simulation with $N_{\text{MC}}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

Time-dependent harmonic oscillator



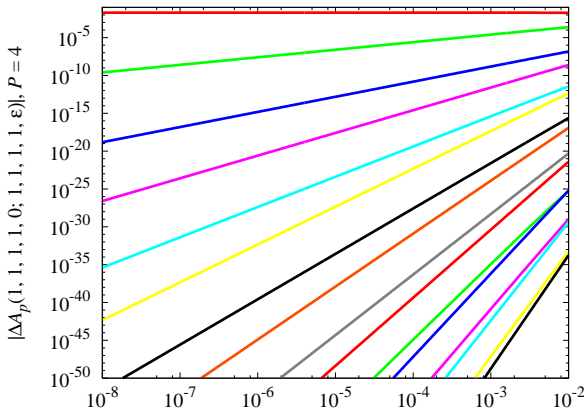
Convergence of discretized amplitudes for the time-dependent harmonic oscillator $V_{G,HO}(x, t) = \frac{\omega^2 x^2}{2(1+t^2)^2}$, with $\omega = 1$ and $p = 2, 4, 6, 8, 10, 12, 14, 16, 18, 20$ (left, top to bottom), and for long time of propagation using MC simulation with $N_{MC} = 2 \cdot 10^9$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

Time-dependent pure quartic oscillator



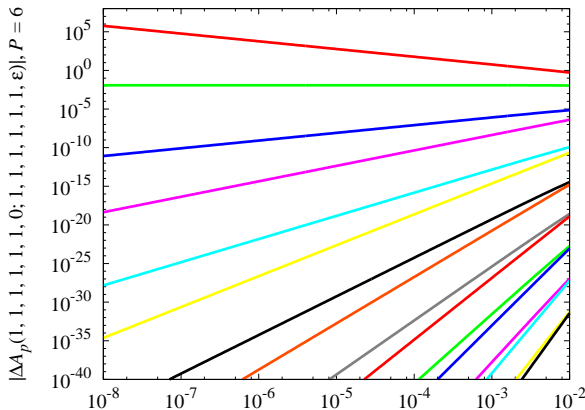
Convergence of discretized amplitudes for the time-dependent pure quartic oscillator $V_{G,PQ}(x, t) = \frac{gx^4}{24(1+t^2)^3}$, with $g = 0.1$ and $p = 1, 2, 3, 7$ (left, top to bottom), and for long time of propagation using MC simulation with $N_{MC} = 1.6 \cdot 10^{13}$ (right).

Many-body example (1)



Errors of numerically calculated amplitudes for a system of four time-dependent harmonic oscillators: $\omega_1^2(t) = 1 + \frac{1}{2} \sin^2 2t$, $\omega_2^2(t) = 1 + \frac{1}{2} \cos 2t$, $\omega_3^2(t) = 2 + \cos 5t$, $\omega_4^2(t) = 4 + \sin^2 4t$.

Many-body example (2)



Errors of numerically calculated amplitudes for a system of six time-dependent harmonic oscillators: $\omega_1^2(t)$, $\omega_2^2(t)$, $\omega_3^2(t)$, $\omega_4^2(t)$, $\omega_5^2(t) = 2 + \sin^2 t$, $\omega_6^2(t) = 4 + 2 \cos 3t$.



Conclusions

- 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 use this approach to study quantum dynamics
 - Evolution in real and imaginary time



Outlook

- Ground states of low-dimensional quantum systems
- Properties of interacting Bose-Einstein condensates
 - Dynamic generation of vortices
- Quantum gases with disorder (Anderson localization)
 - Perturbative and non-perturbative approach
 - Characterization of the Bose-Glass phase transition
- Improved estimators for expectations values
 - Heat capacity, magnetization



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