Fast Converging Path Integrals for Time-Dependent Potentials

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

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

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

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

Approximate calculation of short-time amplitudes leads to

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

Path integral formalism (2)

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

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

- 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

\[
H(p, q, t) = \frac{1}{2} p^2 + V(q, t), \quad \text{(naive) discretized action is}
\]

\[
S_N = \sum_{n=0}^{N-1} \left( \frac{\delta_n^2}{2\epsilon} + \epsilon V(x_n, \tau_n) \right),
\]

where \( \delta_n = q_{n+1} - q_n \), \( x_n = \frac{q_{n+1} + q_n}{2} \), \( \tau_n = \frac{t_n + t_{n+1}}{2} \).
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

\[ S^*(x, \delta; \varepsilon, \tau) = \frac{\delta^2}{2\varepsilon} + \varepsilon W(x, \delta; \varepsilon, \tau) \]
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 $\varepsilon$ [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 $A(a, t_a; b, t_b)$

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

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

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

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

we can obtain the equation for the effective potential $W$. 
Schrödinger’s equation (2)

- The equation for $W$:

$$W + \bar{x} \cdot \bar{\partial} W + \varepsilon \partial_{\varepsilon} W - \frac{1}{8} \varepsilon \partial^{2} W - \frac{1}{8} \varepsilon \bar{\partial}^{2} W$$

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

where $V_{\pm} = V(x \pm \bar{x}, \tau \pm \varepsilon/2)$

- In order to solve it, we use short-time expansion of $W$ in a form of double power series

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

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

$$W_{m+1/2,k}(x, \bar{x}; \tau) = \bar{x}_{i_1} \cdots \bar{x}_{i_{2k+1}} c_{m+1/2,k}^{i_1,\ldots,i_{2k+1}} (x; \tau),$$
After inserting the expansion, we obtain two recursion relations for $W$ coefficients:

\[
8(m + k + 1) W_{m,k} = 8 \frac{\Pi(m, k) (\vec{x} \cdot \partial)^{2k} V^{(m-k)}}{(2k)! (m - k)! 2^{m-k}} + \bar{\partial}^2 W_{m,k+1} + \partial^2 W_{m-1,k}
\]

\[
- \sum_{l,r} \left\{ \partial W_{l,r} \cdot \partial W_{m-l-2,k-r} + \partial W_{l+1/2,r} \cdot \partial W_{m-l-5/2,k-r-1}
\right.
\]

\[
+ \bar{\partial} W_{l,r} \cdot \bar{\partial} W_{m-l-1,k-r+1} + \bar{\partial} W_{l+1/2,r} \cdot \bar{\partial} W_{m-l-3/2,k-r}
\right\},
\]

\[
8(m + k + 2) W_{m+1/2,k} = 8 \frac{(1 - \Pi(m, k)) (\vec{x} \cdot \partial)^{2k+1} V^{(m-k)}}{(2k + 1)! (m - k)! 2^{m-k}} + \bar{\partial}^2 W_{m+1/2,k+1}
\]

\[
+ \partial^2 W_{m-1/2,k} - \sum_{l,r} \left\{ \partial W_{l,r} \cdot \partial W_{m-l-3/2,k-r} + \partial W_{l+1/2,r} \cdot \partial W_{m-l-2,k-r}
\right.
\]

\[
+ \bar{\partial} W_{l+1/2,r} \cdot \bar{\partial} W_{m-l-1,k-r+1} + \bar{\partial} W_{l,r} \cdot \bar{\partial} W_{m-l-1/2,k-r+1}
\right\}.
\]
Recursive relations (2)

- Diagonal coefficients can be directly calculated

\[ W_{m,m} = \frac{1}{(2m + 1)!} (\vec{x} \cdot \partial)^{2m} V, \]
\[ W_{m+1/2,m} = 0. \]

- Off-diagonal coefficients are obtained from recursions using the scheme
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 \( p = 1, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20 \) from top to bottom on the left, and for long time of propagation using MC simulation with \( N_{\text{MC}} = 2 \cdot 10^9 \) on the 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 $p = 2, 4, 6, 8, 10, 12, 14, 16, 18, 20$ from top to bottom on the left, and for long time of propagation using MC simulation with $N_{MC} = 2 \cdot 10^9$ on the right.
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 $p = 1, 2, 3, 7$ from top to bottom on the left, and for long time of propagation using MC simulation with $N_{MC} = 1.6 \cdot 10^{13}$ 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