NUMERICAL EVALUATION OF COHERENT-STATE PATH INTEGRALS WITH APPLICATIONS TO TIME-DEPENDENT PROBLEMS

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We study the application of the coherent-state path integral as a numerical tool for wave-packet propagation. The numerical evaluation of path integrals is reduced to a matrix-vector multiplication scheme. Together with a split-operator technique we apply our method to a time-dependent double-well potential.

1 Introduction and Definitions

Throughout this paper, we will consider a standard Hamiltonian

\[ \hat{H} = \hat{T} + \hat{V} = \frac{\hat{P}^2}{2m} + V(\hat{Q}) \] (1)

for a system with one degree of freedom, described by the momentum operator \( \hat{P} \) and the position operator \( \hat{Q} \).

A coherent state \( |\alpha\rangle \) may be defined by means of harmonic oscillator creation and annihilation operators \( \hat{a}^\dagger \) and \( \hat{a} \), respectively,

\[ \hat{a} := \frac{1}{\sqrt{2\hbar}}(\sqrt{m\omega_0} \hat{Q} + i \frac{1}{\sqrt{m\omega_0}} \hat{P}), \] (2)

through

\[ |\alpha\rangle := \exp(\alpha \hat{a}^\dagger - \alpha^* \hat{a}) |0\rangle, \quad \alpha \in \mathbb{C}, \] (3)

where \( |0\rangle \) is the normalised ground state of the harmonic oscillator \( \hat{H}_0 = \hbar \omega_0 (\hat{a}^\dagger \hat{a} + 1/2) \), and the exponential is a displacement operator. (Note that the frequency \( \omega_0 \), and hence the characteristic length scale \( (\hbar/m\omega_0)^{-1/2} \), is completely arbitrary and can be used as an adjustable parameter.)

The time evolution of a coherent state under \( H_0 \) is simple:

\[ e^{-i\hat{H}_0 t} |\alpha\rangle = e^{-\frac{i\omega_0 t}{2}} |\alpha e^{-i\omega_0 t}\rangle. \] (4)

For an operator \( \hat{A} \) we define the antinormal symbol \( A_- (\alpha) \) implicitly by the relation \( (d^2 \alpha := d \text{Re} \alpha d \text{Im} \alpha) \)

\[ \hat{A} = \int \frac{d^2 \alpha}{\pi} |\alpha\rangle \langle \alpha| A_- (\alpha) \]. \] (5)
By virtue of the generalised Trotter formula
\[
\lim_{N \to \infty} \left( \hat{F}(t/N) \right)^N = e^{-it\hat{H}/\hbar},
\]
where \( \hat{F}(t) \) is any operator-valued function with the two properties
\[
\begin{align*}
\hat{F}(t = 0) &= \mathbb{I} \\
\hat{F}(t = 0) := \lim_{t \to 0^+} \frac{1}{t} \left( \hat{F}(t) - \mathbb{I} \right) &= -i \hat{H}/\hbar
\end{align*}
\]
we are able to define the antinormal coherent-state path integral (ACSPI).

However, to exploit the trivial time development of a coherent state under a harmonic oscillator (eq. 4), we consider \( \hat{F} \) of a generalised split-operator type:
\[
\hat{F}(t) := e^{-i\frac{1}{2\hbar}H_0} \hat{G}(t) e^{-i\frac{1}{2\hbar}H_0}
\]
with an operator \( \hat{G} \) such that (7) holds. We represent \( \hat{G} \) by eq. (5) and define the ACSPI
\[
\langle \alpha | e^{-it\hat{H}/\hbar} | \alpha' \rangle := e^{-i\omega_0 t/2}
\]
\[
\lim_{N \to \infty} \int \frac{d^2\alpha_1}{\pi} \cdots \frac{d^2\alpha_N}{\pi} \prod_{\nu=0}^{N} \langle \alpha_\nu e^{+i\omega_0 t/2} | \alpha_{\nu+1} e^{-i\omega_0 t/2} \rangle \prod_{\nu=1}^{N} G_- (\alpha_\nu; t/N)
\]
\[
\alpha \equiv \alpha_0 e^{+i\omega_0 t/2}, \alpha' \equiv \alpha_{N+1} e^{-i\omega_0 t/2}.
\]
Here we use
\[
\hat{G}(t) := \sum_{n=0}^{K} \frac{(-it)^n}{n!} (\hat{H}_1/\hbar)^n
\]
where \( \hat{H}_1 = V(\hat{Q}) - \frac{m\omega_0^2}{2} \hat{Q}^2 \) is the anharmonic part of the Hamiltonian \( \hat{H} \) and \( K \in \{4, 5, \ldots, 10\} \).

An analogous normal coherent-state path integral may also be defined but will not be considered here.

2 Numerical evaluation

For numerical evaluation of the ACSPI (eq. 9) we have to stop at a finite (Trotter-)number \( N \) of integrations and we perform each integration by a quadrature formula
\[
\int \frac{d^2\alpha}{\pi} f(\alpha) \approx \sum_j w_j f(\alpha_j)
\]
Figure 1. The $Q$-expectation value as a function of time for a particle in the potential of equation (15) is shown. In absence of an external field ($S = 0$) the particle is tunneling through the barrier due to nearly degenerate energy eigenvalues. The destruction of tunneling for $S \neq 0$ is due to degenerate quasi-energies in the Floquet picture.

with fixed sets of abscissas $\alpha_j$ and weights $w_j > 0$, and defining a matrix $P(t/N)$ and a vector $v$ by their elements

$$P_{ij} = \sqrt{w_i w_j} e^{-i \frac{\bar{\hbar}}{\hbar} \langle \alpha_i e^{+i \frac{\bar{\hbar}}{\hbar}} | \alpha_j \rangle} \left[ \langle \alpha_i e^{+i \frac{\bar{\hbar}}{\hbar}} | \psi \rangle - \langle \alpha_i e^{+i \frac{\bar{\hbar}}{\hbar}} | H(t/N) | \psi \rangle \right],$$

and

$$v_j := \sqrt{w_j} \langle \alpha_j | \psi \rangle,$$

the discretized version of a single time step propagation becomes a matrix-vector-multiplication

$$v'_i := \sqrt{w_i} \langle \alpha_i | e^{-i \frac{\bar{\hbar}}{\hbar} H(t/N)} | \psi \rangle \approx \sum_j P_{ij}(t/N) v_j.$$

The vector $v'$ represents the wave packet propagated by the time $t/N$.

For time-dependent potentials we choose the time step small enough to treat the potential as time-independent during the time $t/N$. 
3 Application to tunneling phenomena

We apply our method to a symmetric double well potential with an external time-periodic linear potential:

\[ V(\tilde{Q}) = \frac{m\omega_0^2}{8Q_0^2} \left( \tilde{Q}^2 - Q_0^2 \right)^2 + S \sin(\omega t) \tilde{Q} \]  

(15)

The time-independent case \((S = 0)\) shows the phenomena of tunneling (see fig. 1): A wave packet starting in one well moves through the barrier into the other well. However, Großmann et al. \(^3\) observed that application of a time-periodic linear potential with the right strength \(S\) and frequency \(\omega\) can localize the particle in one well.

In figure 1 we show the \(x\)-expectation value of the wave packet as a function of time. Without external field the particle needs about 2500 elementary (single well) oscillation periods to tunnel from one well to the other. However, application of a field with strength \(S = 0.0031\) and frequency \(\omega = 0.01\) suppresses the tunneling process. It is remarkable that this problem has three different time scales: The vibrational period \(T = 2\pi/\omega_0\) around one minimum, the period \(T = 200\pi/\omega_0\) of the driving force, and the tunneling period \(T \approx 2 \cdot 10^5/\omega_0\). This shows the capability of our method to give reliable results for problems with time scales ranging over several orders of magnitude.

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