Evaluation of coherent-state path integrals in statistical mechanics by matrix multiplication

Bernd Burghardt, Joachim Eicke, and Joachim Stolze
Institut für Physik, Universität Dortmund, 44221 Dortmund, Germany

(Received 29 April 1997; accepted 14 October 1997)

The numerical evaluation of coherent-state path-integral representations for partition functions and other quantities in equilibrium quantum statistical mechanics is discussed. Several coherent-state path-integral schemes are introduced, which differ from each other by the order of approximation and by the operator ordering employed in the high-temperature approximation of the density operator. Simple one-dimensional systems are used to test these schemes. For the harmonic oscillator, finite-dimensional approximations to the coherent-state path integral are calculated analytically and compared to each other and to the real-space path integral. For anharmonic systems, integrations must be approximated by quadrature formulas. This leads to a matrix multiplication scheme which is tested for the double-well potential. The results obtained are accurate from zero temperature way up into the high-temperature regime where quantum effects become negligible. This is a significant advantage over traditional real-space path integral schemes which break down at low temperatures. © 1998 American Institute of Physics. [S0021-9606(98)00704-1]

I. INTRODUCTION

Ever since its invention, path integration has been an important tool of quantum physics. Among its traditional applications in analytic calculations are the development of approximation schemes and perturbation expansions and considerations involving the transition region between classical and quantum physics. During the past two decades roughly, path integration has also found widespread usage¹ as a means of practical numerical calculations of dynamic and thermodynamic quantities. Most of these applications are based on the traditional² real-space path integral involving the Feynman-Kac formula for integration over paths \( \mathbf{r}(t) \) in configuration space.

A less traditional variant of path integration uses coherent states.³⁴ Although the coherent-state path integral has made it into the textbook literature,⁵ it has up to now not found the attention it deserves in its role as a practical numerical tool, with some notable exceptions.⁶–⁸ For numerical purposes, a path integral must be approximated by an \( N \)-dimensional integral (where \( N \) is often called the Trotter number). Quite some time ago one of the present authors studied⁹ finite-\( N \)-approximations to the path-integral representation of the canonical density operator of the harmonic oscillator. It was found that the coherent-state path integral possesses superior convergence properties as compared to the real-space path integral in the case of the harmonic oscillator, where all integrations may be carried out analytically. That superior performance of the coherent-state path integral is due to the fact that the coherent states (in contrast to the position operator eigenstates used in the real-space path integral) have built in the right amount of quantum fluctuations. In the present paper we present the results of the first detailed, systematic numerical study of simple model systems, both harmonic and anharmonic. Our focus will be on the convergence properties of finite-\( N \) approximations to path integral representations of the partition function or free energy.

The plan of the paper is as follows. In Sec. II we fix the notation for the real-space path integral and the coherent-state path integral. In Sec. III we discuss discretized real-space and coherent-state path-integral expressions for the partition function of the harmonic oscillator. In Sec. IV we introduce a simple matrix multiplication scheme which may be used to compute coherent-state path integrals, and in Sec. V we present numerical results for a simple anharmonic system, namely a particle in the double well potential. Section VI concludes the paper.

II. DIFFERENT PATH INTEGRAL PROCEDURES

Throughout this paper, we will consider a standard Hamiltonian

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

(2.1)

for a system with one degree of freedom, described by the momentum operator \( \hat{P} \) and the position operator \( \hat{Q} \). The conventional definition of the path integral starts with the generalized Trotter formula of \( \nu \)th order,

\[
e^{-\beta H} = \left[ f \left( \frac{\beta}{N} \right) + \mathcal{O} \left( \left( \frac{\beta}{N} \right)^{\nu+1} \right) \right]^N.
\]  

(2.2)

A. Real-space path integral

The traditional real-space path integral (RSPI) follows from the first-order Trotter approximation

\[
f \left( \frac{\beta}{N} \right) = e^{-\frac{\beta}{N} \hat{P}^2} e^{-\frac{\beta}{N} \hat{V}} + \mathcal{O} \left( \left( \frac{\beta}{N} \right)^2 \right)
\]  

(2.3)

by inserting \( N \) complete sets each
\begin{equation}
\int_{-\infty}^{\infty} dx |x\rangle \langle x| = \int_{-\infty}^{\infty} dp |p\rangle \langle p| = 1 \tag{2.4}
\end{equation}
of position and momentum eigenstates \( P(p) = p |p\rangle \); \( Q(x) = x |x\rangle \). The \( N \) Gaussian \( p \) integrals may be performed analytically, resulting in the following discretized RSPI representation of the (non-normalized) density operator matrix element between position eigenstates

\[
Q(x,x';N): = \left( \frac{m}{2 \pi \hbar^2 \tau} \right)^N \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_N \\
\times \exp \left[ -\tau \sum_{\nu=1}^{N} \left( \frac{m}{2} \left( \frac{x_{\nu-1} - x_{\nu}}{\hbar \tau} \right)^2 \right) \\
+ V(x_{\nu}) \right] \rightarrow \langle x | e^{-\beta H} | x' \rangle, \tag{2.5}
\]

where

\[
\tau := \beta / N
\]
and \( x_{0} := x \), \( x_{N} := x' \). Replacement of Eq. (2.3) by other Trotter approximations leads to alternative RSPI procedures which may depend differently on \( N \). An example is the choice

\[
f(\tau) = e^{-\frac{\tau}{2} V} e^{-\tau e^{-\frac{\tau}{2} V} + \zeta(\tau)}
\]
which leads to a formula analogous to Eq. (2.5), but with \( V(x_{\nu}) \) ("end point discretization") replaced by \( \frac{\tau}{2}[V(x_{\nu}) + V(x_{\nu-1})] \) ("trapezoidal rule discretization") which performs better\(^{10}\) than Eq. (2.5). Other higher-order Trotter approximations have been discussed by various authors (see, for example, Refs. 11–17).

**B. Coherent-state path integral**

A coherent state\(^{3,4}\) \( |\alpha\rangle \) may be defined by means of harmonic oscillator creation and annihilation operators \( a^\dagger \) and \( a \),

\[
a = \frac{1}{\sqrt{2\hbar}} \left( \sqrt{m \omega} Q + i \frac{1}{\sqrt{m \omega}} P \right),
\]
through

\[
|\alpha\rangle := \exp(\alpha a^\dagger - \alpha^* a)|0\rangle, \tag{2.9}
\]
where \( |0\rangle \) is the normalized oscillator ground state, and the exponential is a displacement operator. \( |\alpha\rangle \) is an eigenstate of the annihilation operator,

\[
a |\alpha\rangle = \alpha |\alpha\rangle \tag{2.10}
\]
and it inherits the minimum-uncertainty property of \(|0\rangle \). [Note that the frequency \( \omega \), and hence the characteristic length scale \((\hbar / m \omega)^{-1/2}\), is completely arbitrary and can be used as an adjustable parameter.] The resolution of unity

\[
\int \frac{d^2\alpha}{\pi} |\alpha\rangle \langle \alpha| = 1 \tag{2.11}
\]

\((d^2\alpha = d\text{Re} \alpha \ d\text{Im} \alpha)\), in combination with the Trotter formula (2.2) obviously offers the opportunity of defining a coherent-state path integral (CSPI). We will use a slightly more general CSPI definition\(^{18}\) employing the normal and antinormal symbols of an operator \( A \). The normal symbol \( A_+(\alpha, \alpha') \) is defined by

\[
A_+(\alpha, \alpha') := \langle \alpha| A |\alpha'\rangle; \tag{2.12}
\]
an obvious way to evaluate it is by normal-ordering the operator \( A \) (i.e., writing \( A \) in terms of \( a^\dagger \) and \( a \) so that in every term all \( a^\dagger \)'s stand to the left of all \( a \)'s) and then [by Eq. (2.10)] replacing \( a^\dagger \) by \( \alpha^* \) and \( a \) by \( \alpha \). The antinormal symbol \( A_-(\alpha) \) is defined by

\[
A = \int \frac{d^2\alpha}{\pi} |\alpha\rangle \langle A |\alpha\rangle \tag{2.13}
\]
and can be obtained by bringing \( A \) into antinormal form (\( a \) left of \( a^\dagger \)) and replacing \( a \) by \( \alpha, a^\dagger \) by \( \alpha^* \). Note that in contrast to \( A_+ \), \( A_- \) depends only on one complex argument. Whereas \( A_+(\alpha, \alpha') \) exists for all practically relevant operators, \( A_- (\alpha) \) is a much more delicate function and it exists only for a restricted class of operators.\(^{21}\)

For \( H = A + B \) and the first-order Trotter approximation

\[
f(\tau) = e^{-\tau A} e^{-\tau B} + \zeta(\tau) = (1 - \tau A)(1 - \tau B) + \zeta(\tau) \tag{2.14}
\]
we can now define the discretized CSPI representation for the matrix element of the (non-normalized) density operator between coherent states

\[
Q(\alpha, \alpha'; N) := \int \frac{d^2\alpha_1}{\pi} \cdots \int \frac{d^2\alpha_N}{\pi} \\
\times \exp \left[ -\tau \sum_{\nu=1}^{N} \left( A_+(\alpha_{\nu-1}, \alpha_{\nu}) \\
+ B_-(\alpha_{\nu}) \right) + \sum_{\nu=1}^{N+1} \frac{\alpha_{\nu}^* - \alpha_{\nu-1}^*}{2\tau} \right] \rightarrow \langle \alpha | e^{-\beta H} | \alpha' \rangle, \tag{2.15}
\]
with \( \alpha_{0} := \alpha, \alpha_{N+1} := \alpha' \). We have used the scalar product of two coherent states

\[
\langle \alpha | \alpha' \rangle = \exp \left[ -\frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2} + \alpha^* \alpha' \right] \tag{2.16}
\]
and the fact that \( 1 - \tau x = \exp(-\tau x) \) to first order in \( \tau \). Equation (2.15) offers a wide variety of CSPI representations for \( \langle \alpha | e^{-\beta H} | \alpha' \rangle \), due to the freedom of choice in the partition \( H = A + B \). Two obvious simple choices are \( B = 0 \), leading to the "normal coherent-state path integral" (NCSIPI), and \( A = 0 \), leading to the "antinormal coherent-state path integral" (ACSPI).\(^{5,6,22}\) Both kinds of CSPI will be discussed in the following sections. We conclude this general section by
pointing out an important potential advantage of the ACSPI: the antinormal symbol of a Hermitian Hamiltonian $H$ is a real-valued function (if it exists at all); this means that the nontrivial part of the exponent in Eq. (2.15) is a real-valued function.

III. HARMONIC OSCILLATOR, ANALYTIC CONSIDERATIONS

The finite-$N$ approximation to the harmonic oscillator partition function resulting from the RSPI prescription (2.5) (the simplest Trotter approximation) is easily calculated:

$$Z_N = \int_{-\infty}^{\infty} dx \varrho(x|x;N) = (\det A)^{-1/2}. \quad (3.1)$$

Here $A$ is a $(N \times N)$ matrix with elements $A_{\nu \nu} = 2 + (\hbar \omega \tau)^2$ and $A_{\nu \nu+1} = A_{\nu \nu-1} = -1$ ($\nu = 0$ to be identified with $\nu = N$). The eigenvalues of $A$ are

$$a_{\nu} = 2 + (\hbar \omega \tau)^2 - 2 \cos \left( \frac{2 \nu \pi}{N} \right) \quad (l = 1, \ldots, N). \quad (3.2)$$

The product of the eigenvalues is known\(^{23}\) and the approximate partition function is

$$Z_N \equiv \left[ 2 \sinh \left( N \sinh \left( \frac{\beta \hbar \omega}{2} \right) \right) \right]^{-1} \quad (3.3)$$

which obviously converges to the exact result for $N \to \infty$. For $\beta \to \infty$ at fixed $N$ (Ref. 24) the approximate free energy $F_N = -\beta \nu$ in $Z_N$ does not converge to the correct ground-state energy $E_0 = \hbar \omega / 2$, but to the “classical ground-state energy” $E = 0$. This phenomenon was called “classical collapse” in an earlier investigation\(^{25}\) of Eq. (3.3). The second-order Trotter approximation (2.7) leads to the same approximate partition function as the first-order formula (2.3) due to cyclic invariance of the trace. For quantities not involving the trace, such as $\varrho(x|x;N)$ (2.7) improves convergence.\(^{10}\) Higher-order Trotter approximations\(^{11}\) lead to an interesting approximation\(^{12,13}\) for the partition function, which looks like the one obtained from Eq. (2.5), but with $V(x)$ replaced by an (temperature-dependent) effective potential

$$V_{\text{eff}}(x) = V(x) + \frac{\hbar^2 \tau^2}{24m} \frac{d}{dx} V, \quad (3.4)$$

which tends to drive the particle away from regions with strong forces as $T$ is lowered. For the harmonic oscillator (3.4) amounts to replacing the natural frequency $\omega$ by an effective frequency

$$\omega_{\text{eff}} = \omega \left[ 1 + \frac{\beta \hbar \omega}{N} \right]^{1/2} \quad (3.5)$$

and consequently inserting $\omega_{\text{eff}}$ into Eq. (3.3) yields the improved approximation to the partition function. Although that leads to a significant improvement, it does not prevent classical collapse.\(^{26}\) This is demonstrated in Fig. 1, where we have plotted the results for the free energy and the partition function according to the approximations (3.3) and (3.5), for both $N = 3$ and $N = 10$. The signs of classical collapse are clearly visible in the main plot. The inset shows that RSPI yields good results at high $T$, as expected.

We now discuss the discretized CSPI representation for the matrix element $\varrho(\alpha, \alpha';N)$ (2.15) for the harmonic oscillator. With $A = xH; B = (1 - x)H$ ($0 \leq x \leq 1$) we obtain

$$A_+ (\alpha_{\nu-1}, \alpha_{\nu}) = x \hbar \omega (\alpha_{\nu-1} \alpha_{\nu} + \frac{1}{2}) \quad (3.6)$$

and

$$B_- (\alpha_{\nu}) = (1 - x) \hbar \omega (|\alpha|^2 - \frac{1}{2}). \quad (3.7)$$

Inserted into Eq. (2.15) this yields

$$\varrho(\alpha, \alpha';N) = \exp \left[ \beta \hbar \omega \left( \frac{1}{2} - x \right) \right] \frac{d^2 \alpha_1}{\pi} \cdots \frac{d^2 \alpha_N}{\pi} \times \exp \left[ -\gamma \sum_{\nu=1}^{N} |\alpha_{\nu}|^2 - \frac{1}{2} (|\alpha_0|^2 + |\alpha_{N+1}|^2) \right. \right.$$  

$$+ \delta \sum_{\nu=1}^{N} \alpha_{\nu}^* \alpha_{\nu} + \alpha_{N+1}^* \alpha_{N+1} \right]. \quad (3.8)$$

Here

$$\gamma = 1 + \frac{\beta \hbar \omega (1-x)}{N}; \quad \delta = 1 - \frac{\beta \hbar \omega x}{N}, \quad (3.9)$$

and $\alpha_0 = \alpha, \alpha_{N+1} = \alpha'$ as in Eq. (2.15). The parameter $x$ allows for continuous interpolation between NCASI ($x = 1$) and ACSPI ($x = 0$). The integrations in Eq. (3.8) may be performed one by one, using the “composition rule”

![Graph](image-url)

Fig. 1. Main plot: free energy of the harmonic oscillator as a function of $T$, for different approximations to the real-space path integral, for $N = 3$ (thin lines) and $N = 10$ (heavy lines). The standard approximation (3.3) is shown dashed, the improved approximation given by (3.5) is shown dot-dashed. The thin solid line shows the exact free energy for comparison. The inset shows the corresponding approximate partition functions, divided by the exact partition function. $F$ and $kT$ are measured in units of $\hbar \omega$.\(^{5\text{a}}\)
However, the NCSPI is seen to give an excellent approximation to the form
\[
\frac{d^2\alpha}{\tau} \left\{ \exp\left(-\frac{\xi_p}{\tau} \alpha_p^2 + \eta_p \alpha_p^2 \right) \right. \\
\times \left. \exp\left(-\frac{\xi_{p+1}}{\tau} \alpha_{p+1}^2 + \eta_{p+1} \alpha_{p+1}^2 \right) \right. \\
= \frac{1}{\xi_p} \exp\left(-\frac{\xi_p}{\tau} \alpha_p^2 + \eta_p \alpha_p^2 \right) \\
\left. \frac{1}{\xi_{p+1}} \exp\left(-\frac{\xi_{p+1}}{\tau} \alpha_{p+1}^2 + \eta_{p+1} \alpha_{p+1}^2 \right) \right) \\
(3.10)
\]
valid for arbitrary positive \( \xi_p \) and \( \eta_p \). This leads to
\[
\mathcal{Q}(\alpha, \alpha'; N) = \frac{1}{\gamma^N} \left\{ \frac{1}{2} |\alpha|^2 - \frac{1}{2} |\alpha'|^2 \right\}^{N/2} \\
\times \left( 1 - \frac{\beta}{\gamma} \right), \\
(3.11)
\]
which converges to the exact density operator matrix element for \( N \to \infty \). The approximate partition function assumes the form
\[
Z_N := \int \frac{d^2\alpha}{\tau} \mathcal{Q}(\alpha, \alpha; N) = \frac{e^{\beta \hbar \omega}}{\gamma^N - \beta^N}. \\
(3.12)
\]
For fixed (even) \( N \) the denominator in Eq. (3.12) has a zero at large \( \beta \) (Ref. 24) for \( \chi > 1/2 \). Nevertheless, the discretized NCSPi may be used for approximate calculations, as Fig. 2 (and earlier examples) shows. For \( \chi < 1/2 \), the approximate free energy does not diverge, but
\[
F_N = -\beta^{-1} \ln Z_N \to -\hbar \left( \frac{1}{\beta} \right). \\
(3.13)
\]
This is the analog of the “classical collapse” observed in the RSPI. Figure 2 displays \( N = 10 \) approximations to the harmonic oscillator free energy from the RSPI (3.3) and the CSPI with \( \chi = 0 \) (ACSPI), 1/2, and 1 (NCSPi). Obviously, none of these schemes reproduces the exact result at low \( T \). However, the NCSPi is seen to give an excellent approximation (to one part in \( 10^3 \) for \( 0.07 \leq kT/\hbar \omega \leq 0.17 \)) over a range of temperatures. A lower bound to that range is defined by the divergence of Eq. (3.12) at \( kT/\hbar \omega = 1/(2N) \) (= 0.05, the left boundary of the inset in Fig. 2). Lower \( T \) may be explored with greater \( N \). For higher \( T \) the RSPI performs better than the CSPI schemes (see inset of Fig. 2, and also Fig. 1).

The success of the NCSPi at low \( T \) may be understood from the fact that \( \alpha = 0 \) is the harmonic oscillator ground state. At low \( T \) the NCSPi thus is dominated by the single path \( \alpha = \text{const} = 0 \), which yields the exact ground-state energy. In a more pictorial language one might say that the coherent states have “built in” the right amount of quantum fluctuations whereas in the RSPI the quantum fluctuations have to be mimicked by integrating over sufficiently strongly fluctuating paths. The paths, however, can only fluctuate sufficiently strongly for a sufficiently fine discretization of the “imaginary time” interval \([0, \beta]\), that is, for sufficiently large \( N \). For given \( N \) the NCSPi thus always yields better low-temperature results than both the RSPI and the ACSPI.

IV. MATRIX MULTIPLICATION SCHEME

For nontrivial Hamiltonians the integrations defining a discretized functional integral have to be performed numerically, that is, by quadrature formulas. It has been observed (in the context of the RSPI) (Refs. 27,28) that these quadratures may be expressed as matrix multiplications, which can be performed very economically by repeatedly squaring a matrix, \( \mathbf{A}^2 \), if the Trotter number is a power of 2. For the NCSPi the matrix multiplication scheme may be formulated as follows. From completeness (2.11) we have the relation
\[
\langle \alpha | e^{-\beta H} | \alpha' \rangle = \int \frac{d^2\alpha''}{\pi} \langle \alpha | e^{-\beta H} | \alpha'' \rangle \langle \alpha'' | e^{-\beta H} | \alpha' \rangle. \\
(4.1)
\]
Using a quadrature formula
\[
\int \frac{d^2\alpha}{\pi} f(\alpha) \approx \sum_i w_i f(\alpha_i) \\
(4.2)
\]
with fixed sets of abscissas \( \alpha_i \) and weights \( w_i > 0 \), and defining a matrix \( \mathbf{P}(\beta) \) by its elements
\[
P_{ij}(\beta) = (w_j) w_i \langle \alpha_j | e^{-\beta H} | \alpha_i \rangle, \\
(4.3)
\]
we obtain from Eq. (4.1) the matrix multiplication formula
\[
P_{ik}(\beta + \beta') = \sum_j P_{ij}(\beta) P_{jk}(\beta'). \\
(4.4)
\]
For the ACSPI a similar scheme is easily derived by replacing \( \langle \alpha | e^{-\beta H} | \alpha'' \rangle \) in Eq. (4.1) with \( e^{-\beta H} | \alpha'' \rangle \langle \alpha'' | e^{-\beta H} | \alpha \rangle \) using the antinormal symbol defined in Eq. (2.13). More general schemes [see Eq. (2.15)] may also be implemented. Equation (4.4) enables us, for example, to evaluate a sequence of approximate partition functions for exponentially decreasing temperature \( T_1, T_2, \ldots, T_N \) by performing \( n \) matrix multiplications. (The subscript of \( Z \) is the Trotter number, as in previous sections.) In order for this scheme to be useful the quadrature formula (4.2) must cover the relevant region in the complex \( \alpha \) plane, it must be sufficiently precise, and it must be sufficiently fast. For the applications discussed here we have chosen quadrature formulas which
treat Re \( \alpha \) and Im \( \alpha \) on equal footing, and which are symmetric about the origin in both variables. Using two indices for notational convenience we may write the abscissas as

\[
\alpha_{rs} := (x_r + iq_s) \quad (r,s = 1, \ldots, 2M + 1)
\]

with

\[
x_r = -x_{2M+2-r}.
\]

The two-dimensional integration is thus expressed as a composition of two identical one-dimensional quadratures.

We have studied two different one-dimensional quadratures, namely an “equidistant” formula, defined by

\[
x_r = \Delta(r - M - 1), \quad w_r = \frac{\Delta}{\sqrt{\pi}},
\]

and a Gauss-Hermite formula designed for integrals of the form

\[
\int_{-\infty}^{\infty} dx e^{-x^2} f(x).
\]

The abscissas and weights for the Gauss-Hermite quadrature may be expressed in terms of Hermite polynomials and can be obtained by standard algorithms. No rescaling of the standard Gauss-Hermite abscissas is necessary, since we can assume that the integrations to be executed [compare Eq. (4.1)] of the form

\[
\int \frac{d^2\alpha''}{\pi} \langle \alpha''|\alpha''\rangle \mathcal{W}(\alpha,\alpha',\alpha'')
\]

with sufficiently smooth \( f \). As Gauss-Hermite quadrature of a given order is exact for integrals like Eq. (4.8) with \( f(x) \) a low-order polynomial, the Gauss-Hermite quadrature should be superior to the equidistant formula (4.7) for smooth functions \( f \) in Eq. (4.9). In practice, however, this advantage of Gauss-Hermite quadrature turns out to be marginal (see Fig. 4 below).

The operation counts and storage requirements for a given number of abscissas are equal for both equidistant and Gauss-Hermite procedures, apart from the determination of the abscissas and weights which has to be performed only once. The matrices \( P \) and \( P^2 \) obviously have \((2M+1)^4\) complex elements each. To compute \( P^2 \) from \( P \), roughly \((2M+1)^6\) complex multiplications and additions have to be performed. Only in fortunate special cases these numbers may reduce significantly due to symmetries. In practice this means that for \( M = 10 \) about 6 megabytes of memory are needed to store \( P \) and \( P^2 \) (assuming 16-byte complex numbers), and a matrix multiplication involves about 86 million complex additions and multiplications, that is, of the order of seconds on a contemporary workstation.

V. NUMERICAL EXAMPLES

In this section we will demonstrate how the matrix multiplication approach suggested in Sec. IV works in practice. Before dealing with anharmonic systems it is useful to take another look at the harmonic oscillator. In the harmonic case, the finite-\( N \) approximation to the CSPI representation of the partition function [in the first-order Trotter approximation (2.14)] is available analytically (3.12) and thus we can study precisely the influence of replacing the intermediate \( \alpha \) integrations in Eq. (3.8) by the quadrature formulas discussed in Sec. IV. The results obtained with an equidistant quadrature formula for the NCSPI at fixed temperature (and fixed Trotter number \( N \)) may be summarized as follows. For a certain range of mesh sizes \( \Delta \) the results for different values of \( M \) ([\((2M+1)^2\) being the number of grid points] coincide with each other and with the analytical result. As \( \Delta \) decreases the results for smaller \( M \) start to deviate from the analytical result first. This is a consequence of the fact that for \( M \) and \( \Delta \) too small the \( \alpha \) region covered by the quadrature formula becomes too small, so that the quadrature formula misses important contributions to the CSPI. As \( \Delta \) grows, the results for all \( M \) values start to deviate from the analytical result simultaneously, because the grid of abscissas for the quadrature formula becomes too coarse. A sufficiently large and fine-meshed grid is given by \( M = 9 \) and \( \Delta = 0.5 \). This value of \( \Delta \) may come as a surprise, since it has been known since John von Neumann’s times\(^4\) that any set of coherent states corresponding to an infinite square grid of \( \alpha \) points with \( \Delta = \sqrt{\pi} \) is overcomplete. It must be kept in mind, however, that \( \{|\alpha_{rs}\rangle\} \) being an overcomplete set does not imply that \((\Delta^2/\pi)\sum_{rs}|\alpha_{rs}\rangle\langle\alpha_{rs}|\) is equal to the unit operator. In a recent analytical study \(^{32}\) Zak showed that only for sufficiently small mesh size does \((\Delta^2/\pi)\sum_{rs}|\alpha_{rs}\rangle\langle\alpha_{rs}|\) approach the unit operator, in accordance with our numerical findings.

We have tested our methods for the quartic anharmonic oscillator, the quartic double-well oscillator, and the (truncated) Morse oscillator. Here we will only discuss results for the quartic double-well oscillator, defined by the potential

\[
V(Q) = \frac{g}{h} m^2 \omega^3 \left( Q - Q_0 \sqrt{\frac{h}{m\omega}} \right)^2 \left( Q + Q_0 \sqrt{\frac{h}{m\omega}} \right)^2,
\]

where \( g \) and \( Q_0 \) are dimensionless parameters. The minima of the double-well potential are situated at the positions \( \pm Q_0 \sqrt{h/(m\omega)} \), the minimum value of the potential energy is zero, and the frequency of small classical oscillations about the minima is \( \Omega = 2 Q_0 \sqrt{g} \omega \) where \( \omega \) is the natural frequency of the harmonic oscillator used to define the coherent states. The height of the barrier between the two minima is \( V(0) = g Q_0^4 \). In our examples we have always chosen the parameter values such that \( \Omega = \omega \).

We have studied ACSPI and NCSPI representations employing Trotter approximations of first and second order. The derivation of the corresponding ordered symbols poses no particular difficulties; starting from the second-order expansion

\[
e^{-rH} = 1 - \tau H + \frac{\tau^2}{2} H^2 + \mathcal{O}(\tau^3),
\]
the operators $H$ and $H^2$ are brought into normal-ordered or antinormal-ordered form, and subsequently the Bose operators are replaced by the appropriate coherent-state variables.

If a Gauss-Hermite quadrature formula is used for the $\alpha$ integrations, the abscissas are fixed as described in Sec. IV. In the case of an equidistant quadrature formula we have fixed the mesh size $\Delta$ according to the following observation. The scalar product $\langle \alpha | \alpha' \rangle = (x + iy)(x' + iy')$ (2.16) contains an oscillatory factor $\exp(\text{i}xy - \text{yx}')$ along with Gaussian factors. The real and imaginary parts of successive $\alpha$ variables in the discretized CSPI thus are related by a Fourier-transform like operation; they exchange their roles in each integration step and consequently should be treated on the same footing. A discretized finite-bandwidth Fourier transform (with kernel $\exp(\text{i}xy)$) between two variables, each capable of $2M + 1$ symmetrically and equidistantly distributed values $(x = \mu \Delta x, y = \mu \Delta y; -M \leq \mu \leq M)$ implies a consistency relation between the spacings $\Delta x$ and $\Delta y$, namely

$$\pi = x_{\text{max}} \Delta y = M \Delta x \Delta y.$$  

(5.3)

In view of the equivalence between $x$ and $y$ discussed above, the natural choice then is

$$\Delta x = \Delta y = \Delta = \sqrt{\frac{\pi}{M}}.$$  

(5.4)

Increasing $M$ thus means both increasing ($\sim M$) the size of the total area covered by the grid and decreasing ($\sim M^{-1}$) the area of each mesh.

In Fig. 3 we display results for the temperature dependent probability density

$$\varrho(x) := \frac{1}{Z} \langle x | e^{-\beta H} | x \rangle$$  

(5.5)

for the double-well potential (5.1) with $x_0 = 5/2$ and $g = 1/50$. The height of the central potential barrier is $\frac{1}{2} \hbar \omega$. The partition function $Z$ may be calculated directly from the CSPI representation of the coherent-state matrix elements of $e^{-\beta H}$, for the calculation of $\langle x | e^{-\beta H} | x \rangle$ we also need the position representation of a coherent state

$$\langle x | \alpha \rangle = \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} \exp \left[ - \left( \frac{m \omega}{2 \hbar} \right)^{1/2} x - \alpha \right]^2 \left( -\text{Im}^2 + \text{Re} \alpha \text{Im} \alpha \right).$$

(5.6)

We have used the ACSPI with second-order Trotter approximation and $\beta \hbar \omega / N = 10^{-3}$. An $M = 7$ equidistant quadrature formula was employed. As the temperature decreases, $\varrho(x)$ develops from a broad featureless distribution (not shown) to the double maximum structure expected at low $T$. As $T$ goes to zero, $\varrho(x)$ approaches the ground-state probability density $|\varphi_0(x)|^2$ obtained from a numerical solution of the Schrödinger equation. The probability density at the origin, $\varrho(0)$, shows a characteristic nonmonotonic behavior (solid line in the inset to Fig. 3). At very high temperatures we expect $\varrho(0)$ to decrease monotonously with growing $T$ as $\varrho(x)$ becomes increasingly broad and flat. This is clearly visible in the left part of the curve. At lower $T$ (that is, $kT$ of the order of the barrier height) the influence of the barrier makes itself felt and $\varrho(0)$ decreases with decreasing $T$, as the double-maximum structure develops. The final increase in $\varrho(0)$ at the very lowest temperatures is easily explained by recalling that the ground-state wave function $\varphi_0(x)$ is an even function with $\varphi_0(0) \neq 0$, whereas the first excited state has $\psi_1(0) = 0$ and therefore does not contribute to $\varrho(0)$. At low $T$ only $\varphi_0$ and $\psi_1$ are appreciably populated, and due to the small energy splitting between these two states it takes very low $T$ to suppress the population of $\psi_1$, thus bringing $\varrho(0)$ up to its asymptotic value $|\varphi_0(0)|^2$.

In spite of the Trotter approximations being essentially high-temperature approximations, the matrix multiplications scheme discussed here is not applicable at arbitrarily high temperatures. The reason for this limitation can be under-
stood from a simple classical consideration; if the region covered by the classical phase space density \( \exp[-\beta H(p,q)]/Z_{\text{cl}} \) [with the classical Hamiltonian \( H(p,q) \)] is not contained well inside the region covered by the quadrature formula, the latter misses important contributions and is bound to fail. For the double-well potential (5.1) a rough estimate may be obtained by computing the values \( q_{\text{max}} \) and \( p_{\text{max}} \) defined by

\[
V(q_{\text{max}}) = \frac{p_{\text{max}}^2}{2m} = kT
\]

and demanding that they be smaller than the values corresponding to the maximum value \( \sqrt{M\pi} \) of both Re \( \alpha \) and Im \( \alpha \). This leads to the following conditions on temperature (numerical values are for \( M = 15 \)):

\[
\beta \hbar \omega > g^{-1}(2M\pi - x_0^2)^{-2} = 6.46 \cdot 10^{-3}, \quad (5.8)
\]

\[
\beta \hbar \omega > (M\pi)^{-1} = 2.12 \cdot 10^{-2}. \quad (5.9)
\]

As discussed above, ‘‘\( > \)’’ is to be interpreted as ‘‘well above’’ here. One might thus suspect that the leftmost part of the solid line in the inset of Fig. 3 should not be taken too seriously. Indeed a classical calculation of \( \mathcal{Q}(0) \) (shown as dot-dashed line), which should be perfectly appropriate for high temperatures, does not agree with the high-temperature part of the quantum calculation with \( M = 7 \). Using \( M = 15 \) (dashed line), however, changes the situation: the quantum and classical calculations then agree for \( \beta \hbar \omega \approx 0.03 \); for smaller \( \beta \) the quantum calculation fails again for the reasons discussed above. However, in that regime, nobody needs a quantum calculation anyway, because the classical calculation becomes exact.

This example demonstrates that the matrix multiplication approach to the approximate evaluation of thermal coherent-state path integrals is able to produce reliable results from zero temperature way up into the classical regime with relatively small effort. This is to be contrasted to the ‘‘classical collapse’’ of the RSPI at low \( T \) discussed in Sec. III above.

We have also calculated the free energy for the double-well potential (with \( x_0 = 5/2 \) and \( g = 1/50 \), as above) in order to see how the choice of the various technical parameters and alternatives in the algorithm influences its performance. In Figs. 4 and 5 we have plotted \( F-F_0 \) as a function of \( \beta \hbar \omega \). \( F_0 \) denotes the exact free energy as calculated from the 300 lowest energy eigenvalues obtained from direct diagonalization. Figure 4 demonstrates (as expected) that the second-order Trotter approximation is far superior to the first-order approximation at low \( T \), whereas the difference between equidistant and Gauss-Hermite quadrature formulas is not significant. (The differences between the two second-order calculations at low \( T \) are fluctuations within the precision range obtainable for the given grid size.)

In Fig. 5 we have plotted the results of eight second-order calculations, using ACSPI (filled symbols) and NCNSPI (open symbols), grid sizes \( M = 11 \) and 13, and \( \beta \hbar \omega \) values of \( 10^{-3} \) and \( 8 \cdot 10^{-3} \). The complete coincidence between open and filled symbols demonstrates that ACSPI and NCNSPI have the same precision. In contrast, \( M \) and \( N \) are important for the precision. Given a sufficiently large grid, choosing a smaller value for the initial imaginary time step \( \beta/N \) leads to a significantly improved precision. This is illustrated by the data sets for grid size \( M = 13 \). Increasing \( N \) is much less expensive than increasing \( M \), because the numerical effort scales as the logarithm of \( N \), but as a power of \( M \). However, if consistently very high precision down to the very lowest temperatures is desired it may be necessary to not only increase \( N \), but also \( M \). This is seen by comparing the \( \beta/N = 10^{-3} \) data sets; the \( M = 11 \) data show a certain loss of precision at very low \( T \), whereas the \( M = 13 \) data saturate at a very high level of precision.

VI. SUMMARY AND CONCLUSIONS

We have discussed the numerical evaluation of coherent-state path integrals for statistical-mechanical quantities. Employing one-dimensional examples, we have demonstrated that discretized coherent-state path integrals can indeed be evaluated with sufficient speed and accuracy by multiple quadratures which in turn may be reformulated as multiple matrix multiplications. This proof of principle is the main result of our paper.

Going into more detail, we have compared the normal and antinormal versions (NCNSPI and ACSPI) of coherent-state path integration, with first- and second-order approximations of the high-temperature density operator, and we have also tried equidistant and Gauss-Hermite quadrature formulas. It seems that the most important factors affecting the accuracy of the results are the order of the approximation and the smallness of the elementary ‘‘imaginary time step’’ \( \beta/N \), given a sufficiently large and fine grid of abscissas in the complex plane for the multiple integrations. Differences in performance between NCNSPI and ACSPI or between equidistant and Gauss-Hermite quadratures seem to be of minor
importance. Similarly, the Gauss-Hermite quadrature performs marginally better than the equidistant one.

Generalization to higher-dimensional problems is possible in principle, but probably difficult in practice, due to the exponential growth in the number of grid points; this is a common disadvantage of all direct evaluation approaches for any kind of path integral. Importance sampling techniques may be applied to reduce the numerical effort per degree of freedom in higher-dimensional problems.

Some of the methods discussed in this paper may also be applied to the calculation of real-time path integrals occurring in quantum dynamics (wave-packet propagation etc.). This is the subject of ongoing research.

ACKNOWLEDGMENTS

This work was supported by the Deutsche Forschungsgemeinschaft through the Schwerpunktprogramm: Zeitabhängige Phänomene und Methoden in der Physik und Chemie. We gratefully acknowledge valuable discussions with Professor Hajo Leschke, Universität Erlangen-Nürnberg, and with members of his group.


