Convergence properties of coherent state path integrals from statistical mechanics

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(Received 6 October 1986; accepted 2 June 1987)

Coherent state path integral representations for matrix elements of density operators are compared to various formulations of coordinate space path integrals discussed recently [R. D. Coalson, J. Chem. Phys. 85, 926 (1986)]. The convergence properties of finite-dimensional approximations to these path integrals are tested for the harmonic oscillator. It is found that at low temperatures the coherent state path integrals converge much better than the coordinate space path integrals and thus should be preferred in numerical (e.g., Monte Carlo) calculations of low-temperature properties.

In a recent contribution¹ to this journal, Coalson discussed properties of various finite-dimensional approximations to path integral expressions from statistical mechanics. Among other topics, he studied the speed of convergence of different computing schemes for matrix elements of the (unnormalized) density operator in position representation

\[ \rho(\beta, x, x') = \langle x | e^{-\beta H} | x' \rangle. \]  

(1)

Path integral expressions for the "thermal propagator" (1) may be derived by using the identity

\[ e^{-\beta H} = \left[ e^{-(\beta/N) H} \right]^N \]  

(2)

and inserting \( N - 1 \) unit operators in the form

\[ 1 = \int d\xi \langle \xi | \xi \rangle \]  

(3)

where \( |\xi\rangle \) denotes a state characterized by a continuous parameter \( \xi \); \( d\xi \langle \xi | \xi \rangle \) is a suitable measure. In the \( N \to \infty \) limit the resulting expression may be viewed as an integral over paths in \( \xi \) space. Normally, \( e^{-(\beta/N) H} \) on the right-hand side of Eq. (2) is replaced by some approximate expression which becomes exact for infinite \( N \).² The usual coordinate space path integral expression for the thermal propagator of the Hamiltonian

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

(4)

(of only one space dimension is considered for notational simplicity) is derived by using

\[ e^{-\beta H} \approx e^{-\beta H_T} e^{-\beta H_N} \]  

(5)

and inserting complete sets of position and momentum eigenstates.³ The Gaussian integrations over the momentum variables may be performed analytically, leaving a \( d^{N-1} x \) integral.

Obviously the limit \( N \to \infty \) cannot be performed explicitly in numerical calculations. Therefore finite-\( N \) approximations of the path integral have to be used for numerical purposes. Such approximations may be constructed by discretizing the paths in \( x \) space in various ways, or by Fourier analyzing the paths and neglecting high-order Fourier coefficients. These possibilities were considered in Ref. 1; performance tests were carried out by calculating finite-\( N \) approximations to \( \rho(\beta, x, x) \) for the harmonic oscillator, the Morse potential, and a double well potential. In the harmonic oscillator case all calculations may be done analytically, whereas for the two anharmonic potentials mentioned the \( d^{N-1} x \) integration has to be performed by Monte Carlo techniques.

In this note I wish to point out an attractive alternative scheme for approximately calculating path integrals, namely by means of coherent states.⁴ The most commonly used type of coherent state may be defined either as an eigenstate of a boson annihilation operator \( a \) with eigenvalue \( \alpha \),

\[ \alpha |\alpha\rangle = \alpha |\alpha\rangle \]  

(6)

(\( \alpha \) is an arbitrary complex number), or as a displaced harmonic oscillator ground state

\[ |\alpha\rangle = \exp(\alpha a^* - \alpha^* a) |0\rangle \]  

(7)

(\( |0\rangle \) denotes the normalized harmonic oscillator ground state). The coherent states are nonorthogonal:

\[ \langle \alpha | \alpha' \rangle = \exp( - \frac{\alpha \alpha' + \alpha^* \alpha'}{2} ) \]  

(8)

and they provide a resolution of unity in the form

\[ 1 = \int d^{2N} \alpha |\alpha\rangle \langle \alpha| \]  

(9)

where \( \int d^{2N} \alpha \) is shorthand for \( \int_{-\infty}^{\infty} d \Re \alpha \int_{-\infty}^{\infty} d \Im \alpha \).

A path integral representation of the thermal propagator (1) may be obtained from the identity

\[ \rho(\beta, x, x') = \int \frac{d^{2N} \alpha_0 \cdots d^{2N} \alpha_N}{\pi} \langle x | \alpha_0 \rangle \times \left( \prod_{i=1}^{N} \langle \alpha_{i-1} | e^{-(\beta/N) H} | \alpha_i \rangle \right) \langle \alpha_N | x' \rangle, \]  

(10)

as usual, by taking the limit of infinite \( N \). The matrix element \( \langle \alpha_{i-1} | e^{-(\beta/N) H} | \alpha_i \rangle \) cannot be calculated exactly in general (except for the harmonic oscillator and other trivial cases) and has to be approximated, e.g., by

3630 J. Chem. Phys. 87 (6), 15 September 1987 0021-9606/87/183630-04$02.10 © 1987 American Institute of Physics
\[ \langle \alpha_{i-1} | e^{-(\beta/N)H} | \alpha_i \rangle \]
\[ \approx \langle \alpha_{i-1} | \left( 1 - \frac{\beta}{N} H \right) | \alpha_i \rangle \]
\[ = \langle \alpha_{i-1} | \alpha_i \rangle \left( 1 - \frac{\beta}{N} \frac{\langle \alpha_{i-1} | H | \alpha_i \rangle}{\langle \alpha_{i-1} | \alpha_i \rangle} \right) \]
\[ \approx \langle \alpha_{i-1} | \alpha_i \rangle \exp \left\{ - \frac{\beta}{N} \frac{\langle \alpha_{i-1} | H | \alpha_i \rangle}{\langle \alpha_{i-1} | \alpha_i \rangle} \right\} \]  
(11)

Equation (11) defines the most popular\(^5\) (and in many cases the most convenient) version of the coherent state path integral. The evaluation of \( \langle \alpha_{i-1} | H | \alpha_i \rangle \) in Eq. (11) may be performed analytically by means of normal-ordering techniques for a wide range of Hamiltonians\(^6\) including the Morse potential and double well systems discussed in Ref. 1. The remaining integrations over \( d^2 \alpha_0 \cdots d^2 \alpha_N \) have to be performed by numerical means, e.g., by Monte Carlo methods.

I shall now concentrate on the harmonic oscillator, deriving an analytical expression for the finite \( N \) approximation to the coherent state path integral representation of the thermal propagator.\(^7\) This approximation will then be compared to the exact propagator and to the approximations given in Ref. 1.

It is to be expected that the coherent state path integral will perform better than the usual coordinate space path integral for high \( \beta \), as the coherent states include the exact harmonic oscillator ground state (\( \alpha = 0 \)) and thus the path \( \alpha \equiv 0 \) will dominate the path integral at low temperature. The same should hold true for other potentials with a parabolic minimum (or several equivalent parabolic minima). In this case, however, the frequency of the harmonic oscillator used to define the coherent states should be adjusted to the frequency of small classical oscillations about the potential minimum, in order to achieve good results. One might even think about using generalized coherent states defined by the action of a displacement operator [cf. Eq. (7)] on the ground state of the potential in question.

The matrix element of \( e^{-(\beta/N)H} \) in approximation (11) is easily evaluated using Eqs. (6) and (8):
\[ \langle \alpha_{i-1} | e^{-(\beta/N)H} | \alpha_i \rangle \approx \exp \left\{ - \frac{1}{2} \delta + \frac{1}{2} | \alpha_{i-1} |^2 + | \alpha_i |^2 \right\} \]
\[ + (1 - \delta) \alpha_{i-1}^* \alpha_i, \]  
(12)

where \( \delta = \beta \hbar / N \). Combining the matrix elements (12) and performing the (Gaussian) \( d^2 \alpha \) integrations, one immediately obtains the finite-\( N \)-approximation to the thermal propagator between two coherent states:
\[ \langle \alpha_0 | e^{-\beta H} | \alpha_N \rangle \approx \exp \left\{ - N \frac{\delta}{2} - \frac{1}{2} | \alpha_0 |^2 \right\} \]
\[ - \frac{1}{2} | \alpha_N |^2 + (1 - \delta) \alpha_0^* \alpha_N. \]  
(13)

The desired approximation to \( \rho(\beta,x,x') \) is now obtained by using the position representation of a coherent state
\[ \langle x | \alpha \rangle = \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} \exp \left\{ - \sqrt{\frac{m \omega}{2 \hbar}} x - \alpha \right\} \]
\[ - \text{Im}^2 \alpha + i \text{Re} \alpha \text{Im} \alpha \]  
(14)

and performing the remaining Gaussian integrations. The result is
\[ \langle x | e^{-\beta H} | x' \rangle \approx \left( \frac{m \omega e^{-\beta \hbar \omega}}{\pi \hbar (1 - \gamma^2)} \right)^{1/2} \]
\[ \times \exp \left\{ - \frac{m \omega}{2 \hbar} \left[ \frac{1 + \gamma^2}{1 - \gamma^2} (x^2 + x'^2) \right. \right. \]
\[ - \frac{4 \gamma^2}{1 - \gamma^2} xx' \left. \right] \right\} \]  
(15)

where \( \gamma = (1 - \beta \hbar \omega / N)^{1/2} \). For \( N \to \infty \) this expression converges to the well-known\(^8\) exact result. In Ref. 1, only the case \( x = x' = 0 \) was considered for simplicity. Defining (analogous to Ref. 1) a quantity \( C_{\text{coh}} \) by
\[ K_N(\beta,0,0) = \rho^{\text{fp}}(\beta,0,0)/C_{\text{coh}}^{\text{fp}}, \]  
(16)

where the superscript \( \text{fp} \) means "free particle", I obtain
\[ C_{\text{coh}} = \frac{1 - \gamma^2}{2 \beta \hbar \omega}. \]  
(17)

The convergence properties of this expression are now compared to those of the corresponding expressions in Ref. 1. In order to give a balanced comparison, one must take into account that for realistic potentials the intermediate \( d^2 \alpha \) integrations in the coherent state approach and the intermediate integrations over position variables or Fourier coefficients in Ref. 1 have to be performed numerically. Hence one should compare approximations containing equal numbers of numerical integrations. In the coherent state approach the computation of \( K_N(\beta,x,x') \) requires \( N + 1 \) complex integrations, whereas in the coordinate space approach, \( N - 1 \) real integrations are required at stage \( N \). Consequently, an \( N \)th stage approximation in the coherent state approach should be compared to a \( (2N + 3) \)th stage approximation from Ref. 1. In Fig. 1, I compare the quantity \( C_{\text{coh}} / C_{\text{ex}} \) to the corresponding quantity in the best ("trapezoidal rule") approximation of Ref. 1. Here \( C_{\text{ex}} \) is defined in analogy to Eq. (16):
\[ C_{\text{ex}} = \left( \frac{\rho(\beta,0,0)}{\rho(\beta,0,0)} \right)^2 = \frac{\sinh^2 \beta \hbar \omega}{\beta \hbar \omega}. \]  
(18)

The curves in Fig. 1 clearly confirm the trend predicted above: for large \( \beta \) the coherent state approximation is superior, whereas for small \( \beta \) the coordinate space approach should be preferred. The coherent state approximation tends to the exact value for \( \beta \to \infty \), whereas the coordinate space approximations of Ref. 1 deviate more and more from the exact value as \( \beta \) grows. This is clearly exhibited in Fig. 2, where the data of Fig. 1 have been plotted as functions of \( N \) for various temperatures.

The superiority of the coordinate space approach for high temperature may be easily explained. The "trapezoidal rule" discretization prescription used in Ref. 1 may be derived from a formula similar to Eq. (5), namely
\[ e^{-(\beta/N)H} \approx e^{-(\beta/2N)V} e^{-(\beta/2N)T} e^{-(\beta/2N)Y} \]
\[ = e^{-(\beta/2N)V} e^{-(\beta/2N)T} e^{-(\beta/2N)Y} e^{-(\beta/2N)Y}. \]

[In fact, as long as only diagonal elements of the density

J. Chem. Phys., Vol. 87, No. 6, 15 September 1987

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operator are computed, the above formula is completely equivalent to Eq. (5) due to the cyclical invariance property of the trace. This formula is correct up to terms of order $B^2/N^2$, as may be seen by applying (twice) the Baker-Campbell-Hausdorff formula

$$e^A e^B = e^{A+B} - 1/2[A,B] + \text{higher order commutators}$$

and expanding the correction term containing the commutator. As the density operator is represented as a product of $N$ factors, the total error is of the order of $B^2/N^2$. On the other hand, the approximation (11) used in the coherent state approach obviously involves an error of the order $B^3/N^3$ in every step, so the total error is of the order $B^3/N$.

Incidentally, the unsatisfactory convergence of the "midpoint rule" discretization procedure observed in Ref. 1 may also be understood by considering the high temperature thermal propagator $\rho(B/N,x,x')$. As discussed above, the trapezoidal rule approximation to this quantity yields an error of the order $B^3/N^3$. The midpoint rule, however, is obtained from the trapezoidal rule by substituting $(B/N)V(x+x')/2$ for $(B/2N)[V(x) + V(x')]$ in the exponential in $\rho(B/N,x,x')$. This substitution in the exponential obviously causes an error of the order $B/N$ which is not necessarily compensated by the errors of neighboring propagator factors [i.e., $\rho(B/N,x',x''$, etc.).

A conspicuous feature of the pictures is the fact that generally $C_{coh}$ is larger than $C_{ex}$, whereas the corresponding

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**FIG. 1.** The quantity $C/C_{ex}$ (defined in the text) is displayed as a function of the dimensionless inverse temperature $\beta\hbar\omega$. The upper set of curves represents $N$th-stage approximations of the type derived in this paper, the lower set of curves represents $(2N+3)$th-stage approximations from Ref. 1, with $N = 3$ (dot-dash), $N = 6$ (short dash), $N = 9$ (long dash), and $N = 12$ (solid line).

**FIG. 2.** Same as Fig. 1, plotted as function of $N$ for different values of $\beta\hbar\omega$, namely, $\beta\hbar\omega = 1$ (solid line), $\beta\hbar\omega = 2$ (long dash), $\beta\hbar\omega = 3$ (short dashed line), and $\beta\hbar\omega = 4$ (dot-dash). Note that convergence (in $N$) becomes increasingly bad with growing $\beta\hbar\omega$ for the lower set of lines, in contrast to the upper set.
quantity $C_{\text{trap}}$ of Ref. 1 is smaller than $C_{\text{ex}}$. This is plausible from the approximations to the matrix elements of $e^{-(B/N)^{1/2}}$ in the two different approaches: in the coherent state approach [cf. Eq. (11)] one essentially replaces the “matrix element of the exponential” by the “exponential of the matrix element,” an operation which is strongly reminiscent of the well-known Jensen inequality\textsuperscript{9}

\[ \langle e^{x} \rangle \geq e^{\langle x \rangle}, \]  

(19)

where the angular brackets denote the expectation value with respect to some averaging procedure. It is well known\textsuperscript{10} that Jensen’s inequality may be used to derive the Peierls-Bogolyubov lower bound to the partition function and thus it seems plausible that a similar approximation leads to a lower bound for $\rho(\beta, x, x)$ (which is one term of the partition function), and thus to an upper bound for the auxiliary quantity $C$.

On the other hand, the usual approximation (5) in coordinate space path integrals resembles the Golden-Thompson inequality\textsuperscript{11}

\[ \text{Tr } e^{-\beta(A + B)} < \text{Tr } (e^{-\beta A/2^p} e^{-\beta B/2^q})^{2^p} \times \text{Tr } (e^{-\beta A/2^p} e^{-\beta B/2^q})^{2^q} \quad (0 < p < q), \]  

(20)

yielding an upper bound to the partition function. In fact, it has been shown\textsuperscript{12} that the discretized coordinate space path integral representation approaches the partition function from above for the type of Hamiltonians discussed here, i.e., kinetic plus potential energy. Of course, this does not strictly imply the monotonicity property for the diagonal element of the density operator apparent in the figures, but it makes this property plausible.

In summary, I have shown that coherent state path integrals are an attractive alternative to coordinate space path integrals for approximate numerical path integral calculations in statistical mechanics,\textsuperscript{13} especially at low temperatures, where it is desirable to have intrinsically well-convergent methods because of the notorious convergence problems of low-temperature Monte Carlo calculations.

**ACKNOWLEDGMENT**

I am grateful to Uwe Brandt for a helpful discussion.

\textsuperscript{2}The resulting version of Eq. (2) is usually called (generalized) “Trotter formula”; several variants of this formula are discussed in H. De Raedt and B. De Raedt, Phys. Rev. A 28, 3575 (1983).
\textsuperscript{3}See, e.g., Chap. 1 of L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley, New York, 1981); the resulting expression is an “endpoint rule” definition in the nomenclature of Ref. 1.
\textsuperscript{4}See J. R. Klauder and B. S. Skagerstam, *Coherent States—Applications in Physics and Mathematical Physics* (World Scientific, Singapore, 1985) for an introduction to the various sorts of coherent states and for reprints of important publications in this field.
\textsuperscript{5}See, for example, Chap. 27 of Schulman’s book (Ref. 3); for different definitions cf. H. Leschke, in *Feynman Path Integrals*, Lecture Notes in Physics (Springer, Berlin, 1979), Vol. 106, p. 435; M. Ciafaloni and E. Onofri, Nucl. Phys. B 151, 118 (1979), and Sec. 1.6 of Ref. 4.
\textsuperscript{7}Similar coherent state path integral representations of the *temporal* propagator between two coherent states for rather general Hamiltonians at most quadratic in creation and annihilation operators were discussed by M. Hillery and M. S. Zubairy, Phys. Rev. A 26, 451 (1982).
\textsuperscript{13}Recently, R. D. Coalsion, D. L. Freeman, and J. D. Doll, J. Chem. Phys. 85, 4567 (1986) published an approach based on a Fourier representation of coordinate space path integrals. They propose, instead of simply truncating the Fourier expansion, to average the potential with respect to the free-particle-like short wavelength fluctuations of the path. In view of the high quality of their results it might be interesting to apply this method to “paths in $\alpha$ space” in order to improve the coherent state path integral formalism.