Uncertainty of path integral averages at low temperature

T. W. Whitfield and John E. Straub

Department of Chemistry, Boston University, Boston, Massachusetts 02215

Burghardt, Eicke, and Stolze [J. Chem. Phys. **108**, 1562 (1998)] have recently presented analytical results for the coherent state path integral (CSPI) approximation to the harmonic oscillator thermal density matrix in a generalized representation. In this work, the variance of the position and momentum operators for the more common Feynman path integral approximation to the density matrix is examined and compared with the results of the generalized CSPI approximation. Both path integral approaches are found to predict minimum uncertainty states at low enough temperatures. Particular attention is given to estimates of internal energy, which can place limits upon the temperature range over which path integral approximations are valid. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1403691]

I. INTRODUCTION

Imaginary-time path integration is an elegant and convenient way to calculate thermodynamic averages for equilibrium (and possibly dynamical[1–3]) properties of quantum mechanical systems. This is particularly evident in computer simulations of many-body systems, since the amount of computation involved does not grow exponentially with the size of the system.

Among the few well-known path integral formulations,[4] Feynman's original real space (RSPI) formulation[5] finds by far the widest application to problems in statistical mechanics.[6–10] A generally appreciated[11] characteristic of finite-N approximations to the full N-dimensional RSPI is the "classical collapse"[12] of some observables in the limit of low temperature. The finite-N approximation to the internal energy of the one-dimensional harmonic oscillator, for example, loses its ground state energy as $T \rightarrow 0$. To mitigate this situation, the dimensionality (number of amplitudes) N of the RSPI may be increased. Increasing N, however, can prove computationally prohibitive.[13]

The coherent state path integral[4,14,15] (CSPI) is an alternative formulation to the RSPI which has been shown to be particularly well suited to study quantum systems at low temperatures. In contrast with the "collapse" behavior of the RSPI, previous CSPI studies of the harmonic oscillator, by Stolze and co-workers,[16,17] have shown that the finite-N approximation to the free energy may improve at lower temperature.

In this note we use both of these path integral formulations to investigate harmonic oscillator observables, like the variance of the position operator, which cannot be calculated from the partition function alone but which require averaging over the density matrix. It is noted that although some RSPI observables "collapse" in the $T \rightarrow 0$ limit, others may "expand," and not go to the classical limit. This behavior is compared with that of the CSPI. Particular focus is given to the position-momentum uncertainty product and to the internal energy, an observable of frequent interest in path integral simulations.

II. REAL-SPACE PATH INTEGRAL AVERAGES

The starting point for any imaginary-time path integral formulation is a functional representation of the statistical density operator. In the position representation, one may write

$$\rho(x,y) = \int dx_1 \cdots dx_{N-1} \prod_{i=1}^{N} \langle x_{i-1} | e^{-\beta H/N} | x_i \rangle, \quad (2.1)$$

where $x = x_0, y = x_N$, and $\beta = 1/kT$. Equation (2.1) is formally exact, but not very useful as it is. To simplify it, we can factor the exponential using a symmetric form of the Trotter product formula[18]

$$e^{-\beta(T+V)/N} = e^{-\beta V/2N} e^{-\beta T/N} e^{-\beta V/2N} + \mathcal{O}\left(\frac{\beta^3}{N^3}\right), \quad (2.2)$$

where $H = T + V$, $T = P^2/2m$, and $V = V(X)$ (upper case X and P indicate operators). Although unsymmetric Trotter factorizations are often used, Eq. (2.2) is preferred since it leaves the density matrix Hermitean. Neglecting the higher order terms, one may follow an established procedure[4] to write a finite-N expression for the density matrix in the position representation

$$\rho(x,y;N) = \int dx_1 \cdots dx_{N-1} \prod_{i=1}^{N} e^{-\beta V(x_{i-1})/2N}$$
$$\times \langle x_{i-1} | e^{-\beta T/N} | x_i \rangle e^{-\beta V(x_i)/2N}$$
$$= \int dx_1 \cdots dx_{N-1} \, dp_1 \cdots dp_N \prod_{i=1}^{N} e^{-\beta V(x_{i-1})/2N}$$
$$\times \langle x_{i-1} | e^{-\beta T/N} | p_i \rangle \langle p_i | x_i \rangle e^{-\beta V(x_i)/2N}$$
$$= \left(\frac{mN}{2\pi\beta\hbar^2}\right)^{N/2} \int dx_1 \cdots dx_{N-1}$$
$$\times \exp\left(-\sum_{i=1}^{N} \left[\frac{mN}{2\beta\hbar^2}(x_{i-1} - x_i)^2 \right.\right.$$
$$\left.\left. + \frac{\beta}{2N}(V(x_{i-1}) + V(x_i))\right]\right). \quad (2.3)$$

The $N \to \infty$ limit of Eq. (2.3) gives the formal path integral, although N must be finite for numerical evaluation. Note that the RSPI expression for $\rho(x,y;N)$, in distinction from the CSPI formula of the following section, involves N analytic integrations over momentum variables (or equivalently, a functional Legendre transformation of the action[19,20]) and is interpreted as a weighted sum on paths in the configuration space.

If we take $V(x) = \frac{1}{2} m \omega^2 x^2$, Eq. (2.3) can be rewritten as

$$\rho(x,y;N) = e^{-(mN/2\beta\hbar^2)(x^2+y^2)} e^{-(\beta m\omega^2/4N)(x^2+y^2)}$$

$$\times \left(\frac{mN}{2\pi\beta\hbar^2} \right)^{N/2} \int d\mathbf{x}^{N-1} e^{(-\mathbf{x}^T \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{x})}, \quad (2.4)$$

where

$$\mathbf{A} = \left(\frac{mN}{\beta\hbar^2} + \frac{\beta m\omega^2}{2N} \right) \mathbf{I} - \left(\frac{mN}{2\beta\hbar^2} \right) \mathbf{S}, \quad (2.5)$$

$$\mathbf{S} = \delta_{i+1,j} + \delta_{i-1,j}, i,j = 1,2,\ldots,N-1, \quad (2.6)$$

$$\mathbf{B} = \left(\frac{mN}{\beta\hbar^2} \right) (x\delta_{i,1} + y\delta_{i,N-1}). \quad (2.7)$$

$\mathbf{I}$ is the identity matrix. The integral in Eq. (2.4) has a known solution,[21] which has been applied to the harmonic oscillator before.[12,22] Making use of the succinct form given by Kauffmann and Rafelski[12] we write down the following solution:

$$\rho(x,y;N) = C \exp[A(x^2+y^2) + Bxy], \quad (2.8)$$

where

$$C = \left(\frac{m\omega \left(1 + \left(\frac{\beta\hbar\omega}{2N} \right)^2 \right)^{1/2}}{2\pi\hbar \sinh\left(2N \sinh^{-1}\left(\frac{\beta\hbar\omega}{2N} \right) \right)} \right)^{1/2}, \quad (2.9)$$

$$A = -\frac{m\omega \left(1 + \left(\frac{\beta\hbar\omega}{2N} \right)^2 \right)^{1/2}}{2\hbar \sinh\left(2N \sinh^{-1}\left(\frac{\beta\hbar\omega}{2N} \right) \right)}$$

$$\times \cosh\left(2N \sinh^{-1}\left(\frac{\beta\hbar\omega}{2N} \right) \right), \quad (2.10)$$

$$B = \frac{m\omega \left(1 + \left(\frac{\beta\hbar\omega}{2N} \right)^2 \right)^{1/2}}{\hbar \sinh\left(2N \sinh^{-1}\left(\frac{\beta\hbar\omega}{2N} \right) \right)}. \quad (2.11)$$

The form of Eqs. (2.8)–(2.11) is very similar to the presentation of Kauffmann and Rafelski,[12] with the difference that the density matrix is symmetric in x and y, due to our choice of Trotter factorization. This is important when calculating averages for operators (e.g., the kinetic energy operator) which are not diagonal in the position representation.

The approximate density matrix, $\rho(x,y;N)$, may be used to calculate moments of X and P. We begin with the partition function
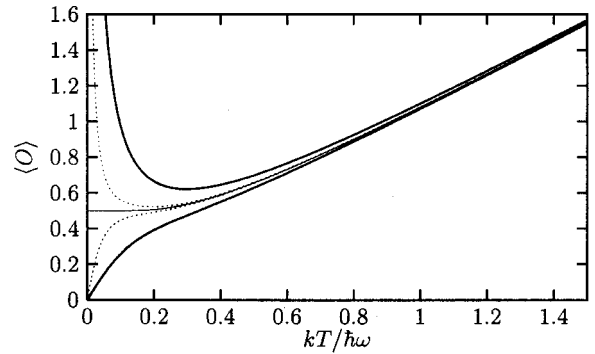

FIG. 1. Real space path integral approximation of $\langle O \rangle$, where $O = m\omega X^2/\hbar$ (curves which "collapse" to the origin at low temperature) or $O = P^2/m\omega\hbar$ (curves which "expand" to infinity at low temperature). The thin line is the exact result, while the bold line corresponds to $N=3$ and the dashed line indicates $N=10$.

$$Z = \int dx\, \rho(x,x;N) = C \sqrt{\frac{\pi}{D}} \quad (2.12)$$

$$= \frac{1}{2} \frac{1}{\sinh\left(N \sinh^{-1}\left(\frac{\beta\hbar\omega}{2N} \right) \right)}, \quad (2.13)$$

where $D \equiv -(2A+B)$. The second moment of the position operator is

$$\langle X^2 \rangle = \frac{1}{Z} \int dx\, x^2 \rho(x,x;N) = \frac{1}{2D} \quad (2.14)$$

$$= \frac{\hbar}{2m\omega} \frac{\coth\left(N \sinh^{-1}\left(\frac{\beta\hbar\omega}{2N} \right) \right)}{\left(1 + \left(\frac{\beta\hbar\omega}{2N} \right)^2 \right)^{1/2}}, \quad (2.15)$$

and of the momentum operator

$$\langle P^2 \rangle = -\frac{\hbar^2}{Z} \int dx \frac{\partial^2}{\partial x^2} \rho(x,y;N) \bigg|_{y=x}$$

$$= -\frac{\hbar^2}{2}(2A-B) \quad (2.16)$$

$$= \frac{m\omega\hbar}{2} \left(1 + \left(\frac{\beta\hbar\omega}{2N} \right)^2 \right)^{1/2} \coth\left(N \sinh^{-1}\left(\frac{\beta\hbar\omega}{2N} \right) \right). \quad (2.17)$$

By symmetry, $\langle X \rangle = \langle P \rangle = 0$.

These results all become exact as $N \to \infty$. With finite N, in the $T \to 0$ limit, however, $\langle X^2 \rangle \to 0$. This is the "classical collapse" behavior observed for the average energy (which is proportional to $\langle X^2 \rangle$, as we shall shortly see) in earlier work.[12] Looking at the momentum in this same limit, $\langle P^2 \rangle \to \infty$. The low temperature limit to the RSPI expression leads to a broadening in the momentum distribution. Both of these moments are drawn in Fig. 1. The uncertainty is

$$\Delta X \Delta P = \sqrt{\langle X^2 \rangle \langle P^2 \rangle} = \frac{\hbar}{2} \coth\left(N \sinh^{-1}\left(\frac{\beta\hbar\omega}{2N} \right) \right), \quad (2.18)$$

which becomes minimal for all N as $T \to 0$. Unlike the *exact* ground state of the harmonic oscillator, however, the minimum uncertainty state approached at low temperature in Eq.

(2.18) is *asymmetric* in the X and P variances. The ground state of the finite-N RSPI belongs to a class of minimum uncertainty states called "squeezed states." [23,24] While ΔX and ΔP are proportional to one another at high temperatures (as they are for all T in the exact case), decreasing the temperature has the effect of squeezing the phase space distribution.

The internal energy may be calculated either from the partition function or by directly averaging over the Hamiltonian,[10,25] generally yielding different estimates of the energy for finite-N and low temperature. The former approach leads to the thermodynamic, or Barker estimator for the energy,

$$E_t = -\partial_\beta \ln Z$$

$$= \frac{\hbar\omega}{2} \frac{\coth\left(N\sinh^{-1}\left(\frac{\beta\hbar\omega}{2N}\right)\right)}{\left(1+\left(\frac{\beta\hbar\omega}{2N}\right)^2\right)^{1/2}} = m\omega^2\langle X^2\rangle, \quad (2.19)$$

while the latter scheme leads to the direct, or Hamiltonian estimator

$$E_h = \frac{1}{Z}\int dx\,dy\,\langle y|H|x\rangle\rho(x,y;N) = \frac{\langle P^2\rangle}{2m} + \frac{1}{2}m\omega^2\langle X^2\rangle. \quad (2.20)$$

The fact that $E_t \neq E_h$ for finite N is equivalent to noting that $\rho(x,y;N)$ is not the exact Green's function for the Bloch equation,

$$\frac{\partial}{\partial\beta}\rho = -H\rho. \quad (2.21)$$

E_t and E_h are, respectively, obtained as the left- and right-hand sides of Eq. (2.21) after taking the trace and dividing by the partition function. Requiring $E_t = E_h$ is therefore a necessary but not sufficient condition that the Green's function of Eq. (2.21) is well approximated by $\rho(x,y;N)$. Accordingly, due to Eq. (2.18), the level of agreement between these two estimators is an indication of the adequacy of N in RSPI simulations. For example, although there has been some concern that the low temperature behavior of E_t might lead to incorrect prediction of phase transitions,[12] use of both E_t and E_h has proven to be an effective safeguard against this.[26] As we shall see in the next section, the situation is more subtle in the CSPI case.

III. COHERENT-STATE PATH INTEGRAL AVERAGES

While the Feynman path integral discussed in the preceding section is certainly the most popular path integral formulation, others have been investigated. The coherent-state formulation, which we focus on presently, and the closely related phase space path integral are both well-known.[4,20] In comparing the low-temperature properties of the RSPI with those of the CSPI, we take a result of Burghardt, Eicke, and Stolze (BES)[17] as our starting point. The following brief background therefore, is merely a guide to direct the reader's attention to certain technical aspects of the discussion (mainly the issue of ordering).

The (canonical) coherent states,[14,27–29] which had an early association with the classical-like dynamics of harmonic oscillator wave packets,[30] were first so-named by Glauber.[31] They can be constructed as eigenstates of the harmonic oscillator annihilation operator:

$$a|\alpha\rangle = \alpha|\alpha\rangle, \quad (3.1)$$

where

$$a \equiv \left(\frac{m\omega}{2\hbar}\right)^{1/2} X + i(2m\hbar\omega)^{-1/2}P. \quad (3.2)$$

The $|\alpha\rangle$ are displaced ground states,

$$|\alpha\rangle = U(\alpha)|0\rangle,$$
$$U(\alpha) \equiv \exp[\alpha a^\dagger - \alpha^* a] = \exp[i(pX - xP)/\hbar], \quad (3.3)$$

where

$$x = \langle\alpha|X|\alpha\rangle = \left(\frac{2\hbar}{m\omega}\right)^{1/2}\mathrm{Re}\,\alpha, \quad (3.4)$$

$$p = \langle\alpha|P|\alpha\rangle = (2m\hbar\omega)^{1/2}\mathrm{Im}\,\alpha. \quad (3.5)$$

Note that since a is not Hermitean, its eigenvalues need not be real. The coherent states are not orthogonal

$$\langle\alpha|\alpha'\rangle = \exp\left[-\frac{|\alpha|^2}{2} - \frac{|\alpha'|^2}{2} + \alpha^*\alpha'\right], \quad (3.6)$$

but do form a complete basis

$$\int \frac{d^2\alpha}{\pi}|\alpha\rangle\langle\alpha| = 1, \quad (3.7)$$

where $d^2\alpha = d\,\mathrm{Re}\,\alpha\,d\,\mathrm{Im}\,\alpha\,(=dx\,dp/2\hbar)$. Actually, since the combination of basis states needed to construct a given superposition is not unique, the coherent states are said to form an *overcomplete* basis. As a consequence of overcompleteness, an operator may be uniquely represented in the coherent state basis in terms only of its diagonal elements.[15,20,24,27,28,32] In particular, the antinormal symbol (or P representation), $O_-(\alpha)$, for an operator O is defined by

$$O = \int \frac{d^2\alpha}{\pi}|\alpha\rangle O_-(\alpha)\langle\alpha|. \quad (3.8)$$

Although O is also unambiguously determined by just the diagonal elements of its normally ordered functional representation, it proves convenient to define

$$O_+(\alpha',\alpha) = \frac{\langle\alpha'|O|\alpha\rangle}{\langle\alpha'|\alpha\rangle}, \quad (3.9)$$

as its normal symbol (Q representation). To underscore the general inequality of these two symbols, note that

$$O_+(\alpha,\alpha) = \int \frac{d^2\alpha'}{\pi}O_-(\alpha')e^{-|\alpha-\alpha'|^2}. \quad (3.10)$$

Finally, the transformation function from the coherent state to the position representation is, to within an arbitrary phase factor,[29]

$$\langle x|\alpha\rangle=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$$

$$\times\exp\left[-\frac{m\omega}{2\hbar}x^2+\left(\frac{2m\omega}{\hbar}\right)^{1/2}\alpha x-\frac{|\alpha|^2}{2}-\frac{\alpha^2}{2}\right].$$

$$(3.11)$$

Just as one does in constructing the RSPI, one may make use of either Eqs. (3.7) and (3.9) or Eq. (3.8) to construct the two well-known CSPI formulations (see, e.g., Ref. 15, pp. 60–74), starting as usual from

$$\rho(\alpha,\alpha';N)=\langle\alpha|(e^{-\beta H/N})^N|\alpha'\rangle.\qquad(3.12)$$

These formulations are, respectively, the normal (NCSPI) and antinormal (ACSPI) coherent-state path integrals, both of which are contained within the following generalized CSPI representation[17,33,34] taken from the work of BES,

$$\rho(\alpha,\alpha';N)=\int\frac{d^2\alpha_1}{\pi}\cdots\frac{d^2\alpha_N}{\pi}\prod_{i=1}^{N+1}\langle\alpha_{i-1}|\alpha_i\rangle\prod_{i=1}^{N}$$

$$\times e^{-\beta(A_+(\alpha_{i-1},\alpha_i)+B_-(\alpha_i))/N},\qquad(3.13)$$

where $\alpha=\alpha_0$, $\alpha'=\alpha_{N+1}$, and $A=\xi H$, $B=(1-\xi)H$ with $0\leq\xi\leq1$.[35] The NCSPI and ACSPI are special cases of Eq. (3.13) where $\xi=1$ and $\xi=0$, respectively. As we shall further explore below, another important special case of Eq. (3.13) is that of symmetric ordering, $\xi=1/2$. Note that because the functional representation of operators in the coherent state basis depends upon ordering [see Eq. (3.10)], the NCSPI and the ACSPI give different approximations to the density matrix, although both become exact as $N\to\infty$.

A. Static approximation ($N=1$)

There are useful thermodynamic inequalities relating to the normal and antinormal CSPI, which place bounds upon the exact value of the partition function in terms of the static approximation ($N=1$):

$$\int\frac{d^2\alpha}{\pi}e^{-\beta H_+(\alpha,\alpha)}\leq\mathrm{Tr}\,e^{-\beta H}\leq\int\frac{d^2\alpha}{\pi}e^{-\beta H_-(\alpha)}.$$

$$(3.14)$$

These are sometimes called the Berezin-Lieb inequalities[15,24,33] and have been applied to the estimation of ground state energies as the low-temperature limit to the free energy.[36]

Before further discussion of the general CSPI approximation to the harmonic oscillator density matrix, we pause to consider the static approximation more closely. If we are interested in the one-dimensional harmonic oscillator, then

$$H_+(\alpha,\alpha)=\hbar\omega\left(|\alpha|^2+\frac{1}{2}\right)=H_{\mathrm{cl}}(x,p)+\frac{\hbar\omega}{2},\qquad(3.15)$$

$$H_-(\alpha)=\hbar\omega\left(|\alpha|^2-\frac{1}{2}\right)=H_{\mathrm{cl}}(x,p)-\frac{\hbar\omega}{2},\qquad(3.16)$$

where $H_{\mathrm{cl}}(x,p)$ is the classical Hamiltonian. [$H_+(\alpha,\alpha)$ is determined using Eqs. (3.9) and (3.1), with H written in terms of normally ordered boson operators (a to the right of $a^\dagger$). After placing H in antinormal order ($a^\dagger$ to the right of a,

using $[a,a^\dagger]=1$), $H_-(\alpha)$ is found by replacing a with α and $a^\dagger$ with $\alpha*$.] The bounds on the exact partition function are

$$Z_\pm=\int\frac{dx\,dp}{2\pi\hbar}e^{-\beta(H_{\mathrm{cl}}(x,p)\pm\frac{\hbar\omega}{2})}=e^{\mp\beta\hbar\omega/2}Z_{\mathrm{cl}},\qquad(3.17)$$

where Z_{cl} is the classical partition function—given by the RSPI for $N=1$. Note that as $\beta\hbar\omega\to0$, $Z_\pm\to Z_{\mathrm{cl}}$. More generally, $Z_\pm\to Z_{\mathrm{cl}}$ as $\hbar\to0$ for any Hamiltonian where $H_\pm=H_{\mathrm{cl}}+\mathcal{O}(\hbar)$.[15] Also note that, from Eqs. (3.15) and (3.16), we expect $Z_\pm$ to carry the prefactor $e^{\mp\beta\hbar\omega/2}$ even for $N>1$, although it will then multiply a function other than Z_{cl}.

Now consider the free energy,

$$F_\pm=-\frac{1}{\beta}\ln Z_\pm=F_{\mathrm{cl}}\pm\frac{\hbar\omega}{2},\qquad(3.18)$$

and the internal energy

$$E_{t,\pm}=-\partial_\beta\ln Z_\pm=E_{\mathrm{cl}}\pm\frac{\hbar\omega}{2}.\qquad(3.19)$$

In the $T\to0$ limit, the static approximation to the NCSPI gives the *exact* ground state energy.[37] As $\beta\to0$, however, where the classical result becomes exact, the free energy and (thermodynamic estimate for) the internal energy are always overestimated (underestimated) for the NCSPI (ACSPI). As we shall see in the next section, this type of behavior, a manifestation of the commutation relation between the boson creation and annihilation operators, is characteristic of the harmonic oscillator ACSPI and NCSPI for all finite N.

For a symmetrically ordered Hamiltonian we have,[38,39]

$$Z_s=\int\frac{d^2\alpha}{\pi}\langle\alpha|e^{-\beta H_s}|\alpha\rangle\qquad(3.20)$$

$$\approx\int\frac{d^2\alpha}{\pi}\langle\alpha|e^{-\beta H_n/2}e^{-\beta H_a/2}|\alpha\rangle\qquad(3.21)$$

$$\approx\int\frac{d^2\alpha}{\pi}e^{-\beta(H_+(\alpha,\alpha)+H_-(\alpha))/2}=Z_{\mathrm{cl}},\qquad(3.22)$$

where $H_s=\frac{1}{2}(H_n+H_a)$, with H_n and H_a the normal and antinormal ordered boson expressions for the Hamiltonian, respectively. Symmetric ordering leads to accurate high temperature behavior.

B. Dynamic paths ($N>1$)

Taking $H=A+B$ as the harmonic oscillator Hamiltonian, the generalized CSPI given above [Eq. (3.13)] can be worked out analytically. BES have found that

$$\rho(\alpha,\alpha';N)=\frac{1}{\gamma^N}\exp\left[-\frac{|\alpha|^2}{2}-\frac{|\alpha'|^2}{2}+\frac{\delta^N}{\gamma^N}\alpha*\alpha'\right.$$

$$\left.+\beta\hbar\omega\left(\frac{1}{2}-\xi\right)\right],\qquad(3.23)$$

where $\delta\equiv[1-(\beta\hbar\omega\xi/N)]$ and $\gamma\equiv(1+[\beta\hbar\omega(1-\xi)/N])$. Using Eqs. (3.11), (3.23), and

$$\rho(x,y;N)=\int\frac{d^2\alpha}{\pi}\frac{d^2\alpha'}{\pi}\langle x|\alpha\rangle\rho(\alpha,\alpha';N)\langle\alpha'|y\rangle,$$

$$(3.24)$$

we can write the CSPI in the form of Eq. (2.8), with

$$C = \left(\frac{m\omega}{\pi\hbar} \right)^{1/2} \frac{e^{\beta\hbar\omega(\frac{1}{2} - \xi)}}{(\gamma^{2N} - \delta^{2N})^{1/2}}, \tag{3.25}$$

$$A = -\frac{m\omega}{2\hbar} \frac{(\gamma^{2N} + \delta^{2N})}{(\gamma^{2N} - \delta^{2N})}, \tag{3.26}$$

$$B = \frac{2m\omega}{\hbar} \frac{\delta^N \gamma^N}{(\gamma^{2N} - \delta^{2N})}. \tag{3.27}$$

All of the results from the preceding section (in terms of A, B, and C) follow:

$$Z = \frac{e^{\beta\hbar\omega(\frac{1}{2} - \xi)}}{\gamma^N - \delta^N}, \tag{3.28}$$

$$\langle X^2 \rangle = \frac{\hbar}{2m\omega} \frac{\gamma^N + \delta^N}{\gamma^N - \delta^N}, \tag{3.29}$$

$$\langle P^2 \rangle = \frac{m\hbar\omega}{2} \frac{\gamma^N + \delta^N}{\gamma^N - \delta^N}, \tag{3.30}$$

$$\Delta X \, \Delta P = \frac{\hbar}{2} \frac{\gamma^N + \delta^N}{\gamma^N - \delta^N}, \tag{3.31}$$

all of which become exact as $N \rightarrow \infty$. Note that the position and momentum distributions are linearly related for all N and T, in distinction from the RSPI case—decreasing the temperature does not squeeze the phase space distribution in the CSPI. Moreover, the uncertainty becomes minimal, and the moments take their ground state values at the zero of δ ($\beta\hbar\omega\xi = N$). This is true also for the ACSPI case, as may be verified by taking the $T \rightarrow 0$ limit.

Equations (3.28)–(3.31) have poles at $kT/\hbar\omega = (\xi - \frac{1}{2})/N$ for N even and $\xi > \frac{1}{2}$. It is therefore natural, our previous discussion of the static approximation to the CSPI notwithstanding, to use this temperature as a lower bound for calculating ($\xi > \frac{1}{2}$) CSPI averages, even for N odd.

Since the essential approximation made in either the normal or antinormal CSPI is a high temperature approximation (i.e., that $e^{-\beta H/N} \approx 1 - \beta H/N$), it is of interest to study these averages at high temperature. Consider the difference between the exact variance (of either position or momentum) and its CSPI approximation,

$$(\Delta X)_{ex}^2 - (\Delta X)_{coh}^2 = \frac{\hbar}{2m\omega} \left(\coth(\beta\hbar\omega/2) - \frac{\gamma^N + \delta^N}{\gamma^N - \delta^N} \right) \tag{3.32}$$

$$\approx \frac{\hbar}{2m\omega} \frac{2\xi - 1}{N} + \mathcal{O}\left(\frac{\beta}{N} \right). \tag{3.33}$$

This result is quite different from a similar expansion for the RSPI averages. In the RSPI case, there is no leading term of zeroth order in β—even for N small, the RSPI averages become exact as $\beta \rightarrow 0$. In order for the CPSI averages to become exact in the high temperature limit, we need either to make N large, or set $\xi = 1/2$. We also note that the ACSPI will overestimate the width of the distribution, while the NCSPI gives an underestimate—just the opposite to what we found earlier for E_t ($N = 1$).
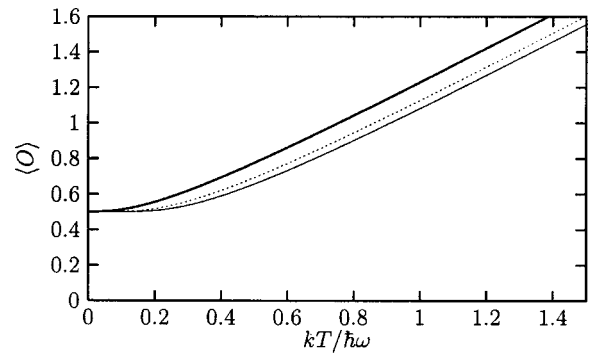
As can be seen in Figs. 2–4, the symmetric ordering

FIG. 2. Coherent state path integral approximation of $\langle O \rangle$, where $O = m\omega X^2/\hbar$ or $O = P^2/m\omega\hbar$. This is an ACSPI ($\xi = 0$) calculation. The thin line is the exact result, while the bold line corresponds to $N = 3$ and the dashed line indicates $N = 10$. The CSPI curves are drawn down to $kT/\hbar\omega = 0$.

scheme ($\xi = 1/2$) appears to give accurate averages not only at high temperatures, but for low temperatures as well. We also see that for N odd and $\xi \neq 0$, the uncertainty may become less than minimal for $kT/\hbar\omega < \xi/N$. This type of low-temperature "classical collapse" behavior is different from what we saw in the RSPI, where although the system may become localized in position, the uncertainty remains at least as great as the minimum predicted by the uncertainty principle.

To compare these three CSPI schemes further, consider the following measure,[40] which gauges how closely the approximate position distribution matches the exact one:

$$\chi^2(\beta, \xi) = \int dx \left(\frac{\rho_{coh}(x,x;N)}{Z_{coh}} - \frac{\rho_{ex}(x,x)}{Z_{ex}} \right)^2 \tag{3.34}$$

$$= \sqrt{\frac{D_{coh}}{2\pi}} - 2\sqrt{\frac{D_{ex}D_{coh}}{\pi(D_{ex} + D_{coh})}} + \sqrt{\frac{D_{ex}}{2\pi}}. \tag{3.35}$$

Looking at Fig. 5, we again see that the choice of $\xi = 1/2$ is optimal over a range of temperatures. The minimum appearing in these figures at $kT/\hbar\omega = \xi/N$ (this will not appear for $\xi = 0$) is due to the zero in δ. Note that χ^2 is increasing for $kT/\hbar\omega < \xi/N$.
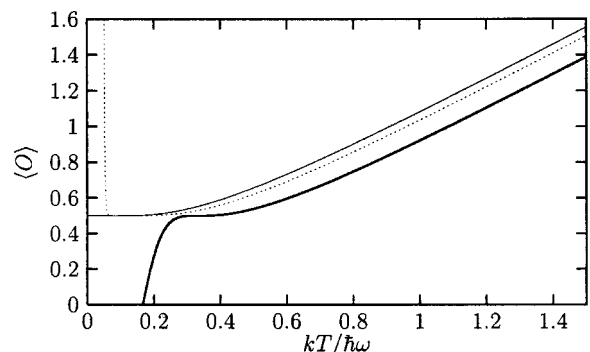

FIG. 3. Coherent state path integral approximation of $\langle O \rangle$, where $O = m\omega X^2/\hbar$ or $O = P^2/m\omega\hbar$. This is a NCSPI ($\xi = 1$) calculation. The thin line is the exact result, while the bold line corresponds to $N = 3$ and the dashed line indicates $N = 10$. The CSPI curves are drawn down to $kT/\hbar\omega = \xi/2N$.
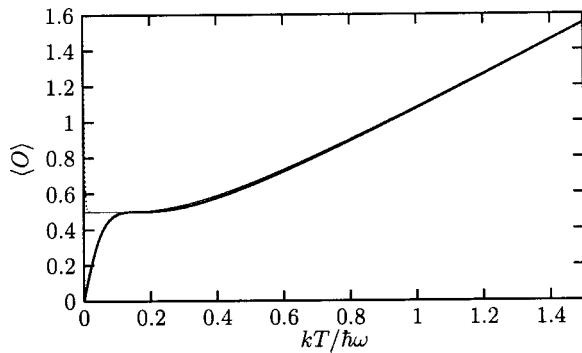
FIG. 4. Coherent state path integral approximation of $\langle O \rangle$, where $O = m\omega X^2/\hbar$ or $O = P^2/m\omega\hbar$. In this calculation, $\xi = 1/2$. The thin line is the exact result, while the bold line corresponds to $N = 3$ and the dashed line indicates $N = 10$. The CSPI curves are drawn down to $kT/\hbar\omega = 0$.

As was the case with the RSPI, there are different schemes to estimate the internal energy. For example,

$$E_t = \hbar\omega \left[\frac{(1-\xi)\gamma^{N-1} + \xi\delta^{N-1}}{\gamma^N - \delta^N} - \left(\frac{1}{2} - \xi\right) \right] \quad (3.36)$$

and

$$E_h = \frac{\hbar\omega}{2} \frac{\gamma^N + \delta^N}{\gamma^N - \delta^N}. \quad (3.37)$$

Both of these energy estimates become exact in the $N \to \infty$ limit. The Hamiltonian estimate of the energy is that of the ground state at $\beta\hbar\omega\xi = N$, but may go below the ground state energy as temperature is further decreased. Since E_h is proportional to the variances, Figs. 2–4 show its behavior. The thermodynamic estimate of the energy is shown in Figs. 6 and 7. In agreement with the low temperature free energy,[17] E_t for the (finite-N) ACSPI goes to $-\hbar\omega/2$ as $T \to 0$.

At *high* temperature, the difference between the exact energy and the Hamiltonian estimate to it is given by Eq. (3.33),

$$E_{ex} - E_h \approx \frac{\hbar\omega}{2} \frac{2\xi - 1}{N} + \mathcal{O}\left(\frac{\beta}{N}\right). \quad (3.38)$$
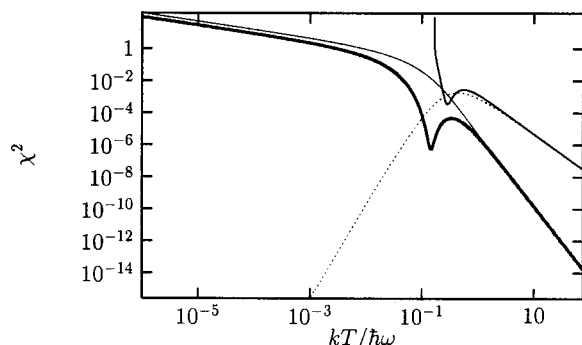

FIG. 5. χ^2 for the RSPI and CSPI approximations to the exact quantum probability distribution. The thinnest line corresponds to the RSPI, the thickest line to the CSPI with $\xi = 1/2$, the dashed line to the ACSPI ($\xi = 0$) and the remaining line to the NCSPI ($\xi = 1$) calculation.
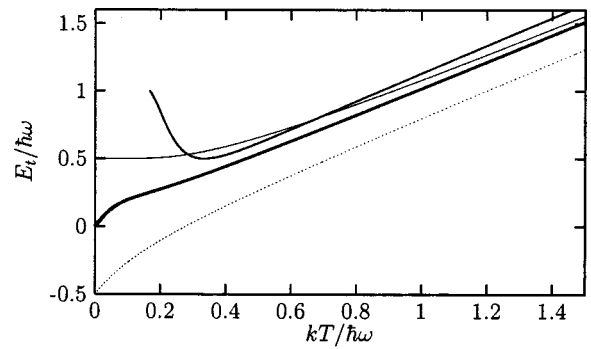

FIG. 6. Coherent state path integral approximations of the internal energy, E_t, calculated from the β derivative of the partition function. The thinnest line corresponds to the exact energy, the thickest line to the CSPI with $\xi = 1/2$, the dashed line to the ACSPI ($\xi = 0$) and the remaining line to the NCSPI ($\xi = 1$) calculation. $N = 3$ throughout. The NCSPI curve is drawn down to $kT/\hbar\omega = \xi/2N$, while the other curves are drawn to $kT/\hbar\omega = 0$.

This difference for the thermodynamic estimate is instead,

$$E_{ex} - E_t = \frac{\hbar\omega}{2} \frac{1 - 2\xi}{N} + \mathcal{O}\left(\frac{\beta}{N}\right). \quad (3.39)$$

To have $E_t = E_h (= E_{ex})$ as $\beta \to 0$, one must either take $N \to \infty$ or use symmetric ordering. At *low* temperatures, however, the NCSPI is known to perform well.[16,17,36] Low temperature agreement between the two energy estimates can confirm this: for $\xi = 1$ and $N > 1$, *both* E_t and E_h go to the ground state energy at $\beta\hbar\omega = N$. Indeed, comparing Figs. 3 and 7, we see that $E_t \approx E_h$ over a range of low temperatures.

By itself however, the requirement that $E_t = E_h$ is generally not as useful for the CSPI as for the RSPI. Looking at Figs. 4 and 7, for example, we see that the symmetrically ordered CSPI trivially satisfies this requirement as $T \to 0$.

IV. DISCUSSION

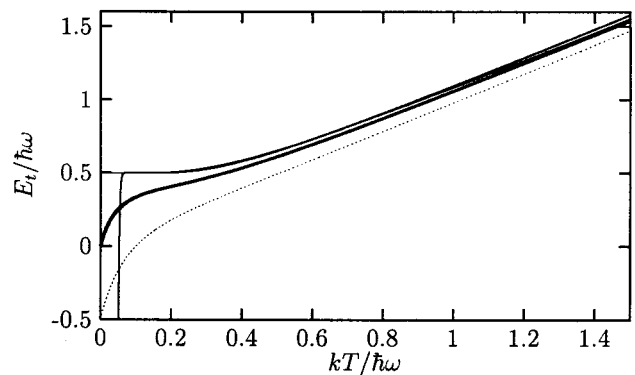We have shown that the "classical collapse" undergone by finite-N approximations to the harmonic oscillator RSPI

FIG. 7. Coherent state path integral approximations of the internal energy, E_t, calculated from the β derivative of the partition function. The thinnest line corresponds to the exact energy, the thickest line to the CSPI with $\xi = 1/2$, the dashed line to the ACSPI ($\xi = 0$) and the remaining line to the NCSPI ($\xi = 1$) calculation. $N = 10$ throughout. The NCSPI curve is drawn down to $kT/\hbar\omega = \xi/2N$, while the other curves are drawn to $kT/\hbar\omega = 0$.

leads to a minimum uncertainty state at low temperatures that is asymmetric in the position and momentum variances. The CSPI variances by comparison, are always proportional to one another, as in the exact case. In the finite-N approximation to the CSPI, the uncertainty becomes minimal at $kT/\hbar\omega = \xi/N$ (which implies zero temperature for the ACSPI). We have seen that if N is not large enough, the minimum uncertainty state will obtain for too high (NCSPI) or too low (ACSPI) a temperature. In the case of the NCSPI (or any representation with $\xi > 1/2$), which may not be defined below $kT/\hbar\omega = \xi/2N$, the uncertainty may become less than minimal in the range $\xi/N > kT/\hbar\omega > \xi/2N$. Symmetric ordering of operators ($\xi = 1/2$) seems to improve this situation, although there is still a ''collapse'' in the uncertainty below $kT/\hbar\omega = \xi/N$.

In the high temperature regime, where RSPI averages are very good, CSPI averages may be poor. We have seen that both the NCSPI and ACSPI schemes imply a constant underestimate or overestimate, respectively, to variances in position and momentum (along with uncertainty and internal energy). This behavior may be understood by noting the effect of reordering the boson operators in the static approximation. Symmetric ordering of the CSPI yields averages which become exact to leading order in β, as they do for the RSPI.

We have discussed different methods to estimate internal energies in path integral calculations. Estimation of internal energies is of frequent interest in path integral computations, whether performed with a numerical matrix multiplication technique,[41,42] which has already been applied to the evaluation of CSPI's,[17] or methods more suitable for many-body problems. In the case of the RSPI, it is convenient to use both E_t and E_h as a check on the adequacy of N—for all finite-N, the two estimates become equal as $\beta \to 0$ and diverge from one another as $\beta \to \infty$. For the CSPI, where the foregoing is generally not true, this approach becomes more subtle. Since equality between E_t and E_h is a necessary, but not sufficient condition for accurately approximating the density matrix, it may happen that the two estimates for the internal energy agree with one another, but not with the exact internal energy. We have noted this situation with the symmetrically ordered CSPI for the harmonic oscillator, as $\beta \to \infty$. Nontrivial agreement between E_t and E_h in CSPI approximations, however, confirms the effectiveness of normal ordering at low temperatures and symmetric ordering at higher temperatures.

In numerical work, the primary advantage of using the coherent state, rather than the more traditional real space formulation of path integrals, comes from the low temperature convergence properties of the NCSPI. With this in mind, it is suggested that agreement between E_t and E_h may serve as a useful guide to identify the *upper* limit of convergence in such calculations. One can also imagine schemes in which agreement between the two energy estimates is maintained by adjusting ξ from 1 to 1/2, as temperature is increased.

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