# Path Integrals and Lower Bounds for Density Matrices 

Eugene P. Gross ${ }^{1}$

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#### Abstract

Feynman has established a variational principle for the coordinate space representation of the canonical density matrix. It uses real trial actions in place of the actual real action. This principle is extended by dividing the original temperature interval, using matrix multiplication, and trial actions that depend on the end points. The result is a series of better lower bounds. A detailed analysis is made of the soluble harmonic oscillator case using free particle and mean path trial actions.


KEY WORDS: Path integrals; density matrices; lower bounds.

## 1. INTRODUCTION

We consider the problem of obtaining lower bounds for the equilibrium density matrix. The point of view is that of Wiener path integrals. ${ }^{(1,2)}$ They are particularly useful in this type of problem, yielding results that are difficult to obtain with conventional quantum mechanics. The approach is developed for the special case of a one-dimensional particle moving in a time-independent potential. Actually these considerations are of much wider validity. They arose in studies ${ }^{(3,4)}$ with multitime actions for polarons, electrons in random potentials, and polymer statistics. The application of the present ideas to these more complicated cases will be described elsewhere.

The starting point is the path integral representation of the density matrix

$$
\begin{equation*}
\rho\left(x_{1} x_{2} \mid \beta\right)=\int_{x(0)=x_{2}}^{x(\beta)=x_{1}} \mathscr{D} x \exp [-S], \quad S=\frac{1}{2} \int_{0}^{\beta} \dot{x}^{2} d u+\int_{0}^{\beta} V(x(u)) d u \tag{1}
\end{equation*}
$$

The basic tool in the analysis of this Wiener integral is the Jensen (convexity) inequality as used by Feynman. Let $S_{0}$ and $S$ be real actions, and introduce the weight function

$$
\begin{equation*}
W_{0}=\exp \left[-S_{0}\right] / r_{0}, \quad r_{0}\left(x_{1} x_{2} \mid \beta\right)=\int_{x(0)=x_{2}}^{x(\beta)=x_{1}} \mathscr{D} x \exp \left[-S_{0}\right] \tag{2}
\end{equation*}
$$

[^0]Then

$$
\begin{equation*}
\rho\left(x_{1} x_{2} \mid \beta\right) \geqslant r_{0}\left(x_{1} x_{2} \mid \beta\right) \exp \left[-\left\langle S-S_{0}\right\rangle_{W_{0}}\right] \tag{3}
\end{equation*}
$$

where ${ }^{2}$

$$
\begin{equation*}
\left\langle S-S_{0}\right\rangle_{W_{0}}=\int_{x_{2}}^{x_{1}} \mathscr{D} x W_{0}\left(S-S_{0}\right) / r_{0}\left(x_{1} x_{2} \mid \beta\right) \tag{4}
\end{equation*}
$$

The simplest choice of $S_{0}$ is the free particle action, which leads to

$$
\begin{align*}
\rho\left(x_{1} x_{2} \mid \beta\right) & \geqslant \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \exp \left[-\Lambda_{0}\left(x_{1} x_{2} \mid \beta\right)\right]  \tag{5}\\
\rho_{0}\left(x_{1} x_{2} \mid \beta\right) & =(2 \pi \beta)^{-1 / 2} \exp \left[-\left(x_{1}-x_{2}\right)^{2} / 2 \beta\right] \tag{6}
\end{align*}
$$

where

$$
\begin{aligned}
\Lambda_{0}\left(x_{1} x_{2} \mid \beta\right) & =\int V(\eta) Q\left(\eta|\beta| x_{1} x_{2}\right) d \eta \\
Q\left(\eta|\beta| \mid x_{1} x_{2}\right) & =\int_{0}^{\beta} d t \rho_{0}\left(x_{1} \eta \mid \beta-t\right) \rho_{0}\left(\eta x_{2} \mid t\right) / \rho_{0}\left(x_{1} x_{2} \mid \beta\right)
\end{aligned}
$$

This can be made the start of a cumulant analysis, which is a useful form of statistical mechanical perturbation theory. However, the lower bound property is lost. One can obtain more accurate bounds by matrix multiplication, since each factor refers to a shorter "time" interval. For example,

$$
\begin{equation*}
\rho\left(x_{1} x_{2} \mid \beta\right)=\int \rho\left(x_{1} y \mid \beta / 2\right) d y \rho\left(y x_{2} \mid \beta / 2\right) \tag{7}
\end{equation*}
$$

since the density matrix depends only on differences of the $\beta$ interval.
Using the free action bound for each half interval, we find

$$
\begin{align*}
\rho\left(x_{1} x_{2} \mid \beta\right) & \geqslant \int d y \rho_{0}\left(x_{1} y \mid \beta / 2\right) \rho_{0}\left(y x_{2} \mid \beta / 2\right) \\
& \times \exp \left\{-\left[\Lambda_{0}\left(x_{1} y \mid \beta / 2\right)+\Lambda_{0}\left(y x_{2} \mid \beta / 2\right)\right]\right\} \tag{8}
\end{align*}
$$

We show explicitly that this is better than the free action bound. Let

$$
\begin{equation*}
W_{0}\left(x_{1} x_{2}|y| \beta\right)=\rho_{0}\left(x_{1} y \mid \beta / 2\right) \rho_{0}\left(y x_{2} \mid \beta / 2\right) / \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \tag{9}
\end{equation*}
$$

be a weight function for the $y$ integration, with fixed values of $x_{1}$ and $x_{2}$. Application of the convexity inequality then leads to the free action bound. The key step in the proof is

$$
\begin{align*}
\int d y & W_{0}\left(x_{1} x_{2}|y| \beta\right) \Lambda_{0}\left(x_{1} y \mid \beta / 2\right) \\
& =\frac{1}{\rho_{0}\left(x_{1} x_{2} \mid \beta\right)} \int_{0}^{\beta / 2} d t \int V(\eta) d \eta \rho_{0}\left(x_{1} \eta \left\lvert\, \frac{\beta}{2}-t\right.\right) \rho_{0}\left(\eta x_{2} \left\lvert\, \frac{\beta}{2}+t\right.\right) \tag{10}
\end{align*}
$$

${ }^{2}$ I am indebted to a referee for pointing out that Jensen's inequality has also been used to get upper bounds on the density matrix; cf. Refs. 6-8. An alternate approach to the problem of lower bounds is found in Ref. 9.
where one uses

$$
\begin{equation*}
\int d y \rho_{0}\left(y x_{2} \mid \beta / 2\right) \rho_{0}(\eta y \mid t)=\rho_{0}\left(x_{2} \eta \left\lvert\, \frac{1}{2} \beta+t\right.\right) \tag{11}
\end{equation*}
$$

The second term in the exponent gives the contribution of the other half of the $\beta$ interval.

For weak potentials one can do the $y$ integration by a cumulant analysis. This shows that the duplication of the free action contains some (but not all) of the higher order perturbation corrections. In compensation, the integrals are simpler than the perturbation formulas. The usefulness of the duplication trick has been pointed out by Miller ${ }^{(5)}$ in connection with a classical path treatment of the diagonal elements of the density matrix. We are exploiting the lower bound feature for the off-diagonal elements and work with simple actions so that the subdivision is feasible.

Using intervals of magnitude $\beta / W$ with $N-1$ integration variables $y, \ldots, y_{N-1}$, we have $\left(y_{0} \equiv x_{1}, y_{N} \equiv x_{2}\right)$

$$
\begin{equation*}
\rho\left(x_{1} x_{2} \mid \beta\right)>\int \prod_{j} \rho_{0}\left(y_{j}-y_{j-1}|\beta| N\right) \exp \left[-\sum_{j=1}^{N} \Lambda_{0}\left(y_{j-1}, y_{j} \mid \beta / N\right)\right] \tag{12}
\end{equation*}
$$

In fact, if the simple free action bound is derived from ordinary quantum mechanics, one has an approach to the construction of the path integral itself. The sequence $y_{1}, \ldots, y_{N-1}$ represents a discrete path. The potential is averaged over a small region for each $y_{j}$. The case of many intermediate steps is analyzed in some detail for the harmonic oscillator in Section 3.

The price one pays for the improved bounds lies in the extra $y_{i}$ integrations. To obtain practical but less accurate bounds one has the flexibility of introducing tractable weight functions $W\left(y_{1} \cdots y_{N-1}\left|x_{1} x_{2}\right| \beta\right)$ containing parameters. The convexity argument is used to find a bound and the parameters are determined by variational considerations. One can then continue with a cumulant analysis of the multiple integral. If there is a classical path for the original path integral of interval $\beta$, this should lead to a preferred set of $y_{j}$ with a fine enough subdivision. Thus far we have only used the free action $S_{0}$ to generate an approximate $\rho\left(x_{1} x_{2} \mid \beta / N\right)$. This $S_{0}$ does not depend directly on the end points $x_{1}, x_{2}$. Clearly, one can consider trial actions of a more general form that depend parametrically on $x_{1}, x_{2}$. This leads to approximations alien to Hamiltonian approaches. This idea can be combined with the subdivision technique. In the next section we examine a mean path action suggested by Feynman and Hibbs. One obtains a bound for each interval that is superior to the free action bound. In Section 3 it is used in a subdivision analysis for the harmonic oscillator.

## 2. MEAN PATH ACTION

We evaluate the density matrix $\rho\left(x_{1} x_{2} \mid \beta\right)$ using a trial action suggested by Feynman and Hibbs. We obtain a better bound for the partition function by bounding the density matrix. The trial action is

$$
\begin{equation*}
S_{0}=\frac{1}{2} \int_{0}^{\beta} \dot{x}^{2} d u+\beta w\left(\bar{x}|\beta| \mid x_{1} x_{2}\right), \quad \bar{x}=\int_{0}^{\beta} x(u) d u \mid \beta \tag{13}
\end{equation*}
$$

It is easy to find the optimal form for $w\left(\bar{x}|\beta| \mid x_{1} x_{2}\right)$. We emphasize that $w$ depends on the end points $x_{1}, x_{2}$ (as well as on $\beta$ ). This action is an example of a typical path integral type of approach. It organizes paths according to their mean position. Paths with the same mean position are assigned the same weight except for the different kinetic energy contributions.

Using a weight $W_{0}$ associated with $S_{0}$, we have

$$
\begin{equation*}
W_{0}\left(x_{1} x_{2} \mid \beta\right)=\exp \left[-S_{0}\left(x_{1} x_{2} \mid \beta\right)\right] / \int_{x_{2}}^{x_{1}} \mathscr{D} x \exp \left[-S_{0}\right] \tag{14}
\end{equation*}
$$

Write the denominator as

$$
\begin{equation*}
\int_{x_{2}}^{x_{1}} \mathscr{D} x \exp \left[-S_{0}\right]=\int d \xi G\left(\xi|\beta| \mid x_{1} x_{2}\right) \exp \left[-\beta w\left(\xi|\beta| \mid x_{1} x_{2}\right)\right] \tag{15}
\end{equation*}
$$

where

$$
\begin{equation*}
G\left(\xi|\beta| \mid x_{1} x_{2}\right)=\int_{x_{2}}^{x_{1}} \mathscr{D} x \exp \left[-\frac{1}{2} \int_{0}^{\beta} \dot{x}^{2} d u\right] \delta(\bar{x}-\xi) \tag{16}
\end{equation*}
$$

This path integral has the explicit form

$$
\begin{equation*}
G\left(\xi|\beta| \mid x_{1} x_{2}\right)=\sqrt{12} \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \exp \left[-\frac{6}{\beta}\left(\xi-\frac{x_{1}+x_{2}}{2}\right)^{2}\right] \tag{17}
\end{equation*}
$$

We also need the path integral

$$
\begin{align*}
T\left(\xi|\beta| \mid x_{1} x_{2}\right) & =\int_{x_{2}}^{x_{1}} \mathscr{O} x \exp \left[-\frac{1}{2} \int_{0}^{\beta} \dot{x}^{2} d u\right] \delta(\bar{x}-\xi) \int_{0}^{\beta} V(x(u)) d u \\
& \equiv \int V(\eta) R\left(\xi|\eta| \beta\left|\mid x_{1} x_{2}\right)\right. \tag{18}
\end{align*}
$$

The function $R$ is listed in the Appendix.
A functional variation with respect to $w\left(\xi|\beta| x_{1} x_{2}\right)$ leads to the simple result

$$
\begin{equation*}
\rho\left(x_{1} x_{2} \mid \beta\right) \geqslant \int d \xi G\left(\xi|\beta| \mid x_{1} x_{2}\right) \exp \left[-\beta w\left(\xi|\beta| \mid x_{1} x_{2}\right)\right] \tag{19}
\end{equation*}
$$

Here

$$
\begin{equation*}
w\left(\xi|\beta| \mid x_{1} x_{2}\right)=T\left(\xi|\beta| \mid x_{1} x_{2}\right) / G\left(\xi|\beta| \mid x_{1} x_{2}\right) \tag{20}
\end{equation*}
$$

This yields a better bound than using the free action. To recover the latter result, use a weight

$$
\begin{equation*}
p\left(\xi|\beta| \mid x_{1} x_{2}\right)=G\left(\xi|\beta| \mid x_{1} x_{2}\right) / \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \tag{21}
\end{equation*}
$$

The convexity bound applied to the $\xi$ integration then yields

$$
\begin{equation*}
\rho\left(x_{1} x_{2} \mid \beta\right) \geqslant \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \exp \left[-\beta \int p(\xi) w(\xi) d \xi\right] \tag{22}
\end{equation*}
$$

Since

$$
\begin{align*}
& \int p(\xi) w(\xi) d \xi \\
& \quad=\int T\left(\xi|\beta| \mid x_{1} x_{2}\right) d \xi / \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \\
& \quad=\int_{x_{2}}^{x_{1}} \mathscr{D} x \exp \left(-\frac{1}{2} \int_{0}^{\beta} \dot{x}^{2} d u\right) \int_{0}^{\beta} V(x(u)) d u / \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \tag{23}
\end{align*}
$$

this is the free action result. One could improve this (at the cost of losing the bound property) by making a cumulant analysis for the $\xi$ integration. The mean path action picks up some (but not all) of the $V^{2}$ corrections.

To obtain results for strong potentials, one should do the $\xi$ integration exactly. This may be difficult. To obtain approximate bounds, introduce a weight function

$$
\begin{equation*}
p_{0}\left(\xi|\beta|\left|x_{1} x_{2}\right|=\exp \left[-\beta w_{0}\left(\xi|\beta| \mid x_{1} x_{2}\right)\right] G\left(\xi|\beta| \mid x_{1} x_{2}\right) / K_{0}\left(x_{1} x_{2} \mid \beta\right)\right. \tag{24}
\end{equation*}
$$

where

$$
K_{0}\left(x_{1} x_{2} \mid \beta\right)=\int d \xi_{1} G\left(\xi_{1}\right) \exp \left[-\beta w_{0}\left(\xi_{1}\right)\right]
$$

Write

$$
\begin{equation*}
\rho\left(x_{1} x_{2} \mid \beta\right) \geqslant \int K_{0}\left(x_{1} x_{2} \mid \beta\right) \int d \xi p_{0} \exp \left[\beta\left(w_{0}-w\right)\right] \tag{25}
\end{equation*}
$$

and apply the convexity bound using $p_{0}(\xi)$. This yields

$$
\begin{equation*}
\rho\left(x_{1} x_{2} \mid \beta\right) \geqslant K_{0}\left(x_{1} x_{2} \mid \beta\right) \exp \left\{\beta \int\left(w_{0} G-T\right) \exp \left(-\beta w_{0}\right) d \xi\right\} \tag{26}
\end{equation*}
$$

Thus, for this case, the procedure of taking an approximate weight function is equivalent to using a trial action $w_{0}\left(\bar{x}|\beta| \mid x_{1} x_{2}\right)$ in place of the optimal $w\left(\bar{x}|\beta| \mid x_{1} x_{2}\right)$.

Let us consider the evaluation of the partition function. The mean path bound is

$$
\begin{equation*}
Z(\beta) \geqslant \int d x_{1} \int d \xi G\left(\xi|\beta| \mid x_{1} x_{1}\right) \exp \left[-w\left(\xi|\beta| \mid x_{1} x_{1}\right)\right] \tag{27}
\end{equation*}
$$

If the potential has continuum states, the integration over $x_{1}$ leads to contributions that depend on the size of the system. Consider the case (such as a harmonic oscillator) where there are only bound states. We exhibit the relation to the way Feynman and Hibbs use their mean path action. Their result is obtained by doing the $x_{1}$ integration first, using the convexity bound, with a weight function

$$
\begin{equation*}
p\left(\xi \mid x_{1}\right)=G\left(\xi \mid x_{1}\right) / l_{0}, \quad l_{0}=\int G\left(\xi \mid x_{2}\right) d x_{2}=(2 \pi \beta)^{-1 / 2} \tag{28}
\end{equation*}
$$

This of course weakens the bound. We find

$$
\begin{equation*}
Z>l_{0} \int d \xi \exp \left[-l_{0}^{-1} \int_{0}^{0} D_{\beta} y \int_{0}^{\beta} V(y(u)+\xi-\bar{y}) d u\right] \tag{29}
\end{equation*}
$$

which is the Feynman-Hibbs result.
The subdivision technique may of course be applied together with the mean path bound. From Eq. (19) one sees that there are $\xi_{j}$ integrations along with the $y_{j}$ integrations of matrix multiplication.

## 3. APPLICATION TO THE HARMONIC OSCILLATOR

To obtain a clearer idea of what the improved bounds are like, consider the exactly soluble case of a harmonic oscillator of unit mass and angular frequency $\omega_{0}$. We use units where $\hbar=1$ and measure lengths in terms of the thermal de Broglie length $1 / \sqrt{ }$. Then $\omega \equiv \omega_{0} \beta$ and the "time" unit is 1 . The exact density matrix for $N$ units is

$$
\begin{equation*}
\rho\left(x_{1} x_{2} N\right)=\bar{F}_{N}(\omega) \exp \left[-\bar{\alpha}_{N}\left(x_{1}{ }^{2}+x_{2}{ }^{2}\right)+\bar{B}_{N} x_{1} x_{2}\right] \tag{30}
\end{equation*}
$$

where

$$
\begin{equation*}
\bar{F}_{N}=\left(\frac{\omega}{2 \sinh \omega N}\right)^{1 / 2}, \quad \bar{\alpha}_{N}=\frac{\omega}{2} \operatorname{coth} \omega N, \quad \bar{B}_{N}=\omega \operatorname{csch} \omega N \tag{31}
\end{equation*}
$$

The partition function is

$$
\begin{equation*}
\bar{Z}_{N}(\omega)=\left(2 \sinh \frac{1}{2} \omega N\right)^{-1}=e^{-\omega N / 2} \sum_{j=0} e^{-j N \omega} \tag{32}
\end{equation*}
$$

The bar indicates that we deal with the exact result.

It is easy to show that both the free action and mean path action lead to density matrices of the above form with approximate values of $\alpha_{N}, B_{N}$, $F_{N}(\omega)$. We are interested in studying the effect of subdividing a given $\omega$ by $N-1$ intermediate steps. Introduce

$$
\begin{equation*}
B_{N} *(\omega)=N B_{N}(\omega / N), \quad \alpha_{N}^{*}=N \alpha_{N}(\omega / N) \tag{33}
\end{equation*}
$$

For the exact solution $\bar{B}_{N}{ }^{*}(\omega)=\bar{B}_{1}(\omega)$ and $\bar{\alpha}_{N}{ }^{*}=\bar{\alpha}_{1}(\omega)$. For the approximate density matrices we see how close $B_{N}{ }^{*}(\omega)$ comes to $B_{1}(\omega)$.

For a density matrix of the above form one has the recurrence formulas

$$
\begin{array}{lr}
\alpha_{N+1}=\alpha_{N}-\left[B_{N}^{2} / 4\left(\alpha_{N}+\alpha_{1}\right)\right], \quad B_{N+1}=B_{N} B_{1} / 2\left(\alpha_{N}+\alpha_{1}\right) \\
F_{N+1}=F_{N} F_{1} \pi^{1 / 2} /\left(\alpha_{N}+\alpha\right)^{1 / 2}, \quad Z_{N}=\pi^{1 / 2} F_{N} /\left(2 \alpha_{N}-B_{N}\right)^{1 / 2} \tag{35}
\end{array}
$$

To reduce this to a convenient form, introduce

$$
\begin{equation*}
A_{N}=\alpha_{N}+\alpha_{1}, \quad \xi_{N}=2 A_{N} / B_{N} \tag{36}
\end{equation*}
$$

Then

$$
\begin{equation*}
\beta_{N+1}=B / \xi_{N}, \quad A_{N+1}=A_{N}\left(1-1 / \xi_{N}^{2}\right) \tag{37}
\end{equation*}
$$

The $\xi_{N}$ generate all of the desired quantities. They obey the two-term recurrence relation

$$
\begin{equation*}
\xi_{N+1}=\left(\xi_{N}^{2}-1\right) / \xi_{N-1}, \quad \xi_{0}=1, \quad \xi_{1}=2 A_{1} / B_{1} \tag{38}
\end{equation*}
$$

The first few values are
$\xi_{2}=\xi_{1}{ }^{2}-1, \quad \xi_{3}=\xi_{1}\left(\xi_{1}{ }^{2}-2\right), \quad \xi_{4}=\left[\xi_{1}{ }^{2}\left(\xi_{1}{ }^{2}-2\right)^{2}-1\right] /\left(\xi_{1}{ }^{2}-1\right)$

The starting point for the free action bound is

$$
\begin{equation*}
\alpha_{1}=\frac{1}{2}\left(1+\omega^{2} / 3\right), \quad B=1-\omega^{2} / 6 \tag{40}
\end{equation*}
$$

The exact $\bar{B}_{1}$ is positive and lies between one and zero. The free action bound gives a negative $B_{1}$ for $\omega>\sqrt{6}$. The $A_{N}{ }^{*}$ and $B_{N}{ }^{*}$ are ratios of polynomials in $\omega^{2}$. For small $\omega$ the exact expansion is

$$
\begin{equation*}
\bar{B}^{-1}=(\sinh \omega) / \omega=\left\{1+\omega^{2} / 6+\bar{\delta} \omega^{4} / 36+\cdots\right\}, \quad \bar{\delta}=3 / 10 \tag{41}
\end{equation*}
$$

The subdivisions with free action bounds yield the sequence

$$
\begin{equation*}
B_{N}^{*-1}=\left\{1+\omega^{2} / 6+\delta_{N}^{*} \omega^{4} / 36+\cdots\right\} \tag{42}
\end{equation*}
$$

The coefficient of $\omega^{2}$ is exact in every approximation. We find
$\delta_{1}{ }^{*}=1, \quad \delta^{2 *}=7 / 16=0.44, \quad \delta^{3 *}=29 / 81=0.36, \quad \delta^{4 *}=85 / 256=0.33$
approaching $\bar{\delta}=0.30$.

The starting point of the mean path theory is

$$
\begin{equation*}
\alpha_{1}=\frac{1}{2}\left(1+\frac{\omega^{2}}{3}-\frac{\omega^{4}}{48} \frac{1}{1+\omega^{2} / 10}\right), \quad B_{1}=1-\frac{\omega^{2}}{6}+\frac{\omega^{4}}{48} \frac{1}{1+\omega^{2} / 10} \tag{44}
\end{equation*}
$$

$B_{1}$ remains positive until $\omega \sim \sqrt{20}$. We find the rapid convergence

$$
\begin{equation*}
\delta_{1}^{*}=1 / 4=0.25, \quad \delta_{2}^{*}=19 / 64=0.298 \tag{45}
\end{equation*}
$$

There are corresponding results for the partition function. We define

$$
\begin{equation*}
Z_{N}(\omega)=Z_{N}(\omega / N) \tag{46}
\end{equation*}
$$

which equals $Z_{1}(\omega)$ for the exact solution. This is

$$
\begin{align*}
& \bar{Z}_{N}(\omega)=1 /[2 \sinh (\omega N / 2)]  \tag{47}\\
& \bar{Z}_{1}(\omega) \rightarrow \omega^{-1}\left\{1-\omega^{2} / 24+\omega^{4}(7 / 360 \cdot 16)+\cdots\right\} \tag{48}
\end{align*}
$$

The free particle action starts with

$$
\begin{align*}
F_{1} & =\left[\exp \left(-\omega^{2} / 12\right)\right] /(2 \pi)^{1 / 2}  \tag{49}\\
Z_{1}(\omega) & =\exp \left(-\omega^{2} / 12\right) / \omega \rightarrow \omega^{-1}\left\{1-\omega^{2} / 12+\omega^{4} / 2(12)^{2}+\cdots\right\} \tag{50}
\end{align*}
$$

The free particle action is wrong by a factor of 2 for the coefficient of $\omega^{2}$. This can be traced to the fact that one needs $2 \alpha_{1}-B_{1}$ correct to order $\omega^{4}$ in order to obtain $Z_{1}(\omega)$ to order $\omega^{4}$. Bisection of the free particle action yields

$$
\begin{align*}
Z_{2} & =\exp \left(-\omega^{2} / 24\right) / \omega\left(1+\omega^{2} / 48\right)^{1 / 2}  \tag{51}\\
& \rightarrow \omega^{-1}\left\{1-\frac{5}{4} \omega^{2} / 24+1.5 \times 10^{-3} \omega^{4}+\cdots\right\} \tag{52}
\end{align*}
$$

which exhibits the improvement in the $\omega^{2}$ coefficient.
The mean path action starts with

$$
\begin{align*}
F_{1}(\omega) & =\left[\exp \left(-\omega^{2} / 30\right)\right] /(2 \pi)^{1 / 2}\left(1+\omega^{2} / 10\right)^{1 / 2}  \tag{53}\\
Z_{1}(\omega) & =\exp \left(-\omega^{2} / 30\right) / \omega\left(1+\omega^{2} / 60\right)^{1 / 2}  \tag{54}\\
& \rightarrow \omega^{-1}\left\{1-\omega^{2} / 24+\omega^{4}(3 / 3200)+\cdots\right\} \tag{55}
\end{align*}
$$

The coefficient of $\omega^{2}$ is correct. The coefficient of $\omega^{4}$ is $9.4 \times 10^{-4}$. The exact coefficient is $12.1 \times 10^{-4}$. Bisecting the interval leads to

$$
\begin{equation*}
Z_{2}^{*}(\omega)=\exp \left(-\omega^{2} / 60\right) / \omega\left[\left(1+\omega^{2} / 40\right)\left(1+\omega^{2} / 48\right)\left(1+\omega^{2} / 240\right)\right]^{1 / 2} \tag{56}
\end{equation*}
$$

The coefficient of $\omega^{4}$ is now $11.2 \times 10^{-4}$.

## 4. CONCLUSIONS

We have shown that a series of lower bounds may be obtained by bounding the off-diagonal coordinate space elements of the density matrix and using matrix multiplication to divide the original interval. The accuracy of the bounds is of course contingent on the choice of the trial action, which in general depends parametrically on the end points. In particular the actions used here are not powerful enough to describe the discrete state structure (cf. the example of the harmonic oscillator). However, the technique can be extended to classical path approximations, as has been pointed out by Miller. ${ }^{(5)}$

## APPENDIX. LIST OF PATH INTEGRALS

The interval is 0 to $\beta$ and $\bar{x}=\beta^{-1} \int_{0}^{\beta} x(u) d u$. We use the abbreviations

$$
D x=\mathscr{D} x \exp \left(-\frac{1}{2} \int_{0}^{\beta} \dot{x}^{2} d u\right), \quad l_{0}=(2 \pi \beta)^{-1 / 2}, \quad s=(t / \beta)(1-t / \beta)
$$

We have

$$
\begin{align*}
F_{0}(k \mid \beta)= & \int_{0}^{0} D x \exp (i k \bar{x})=l_{0} \exp \left(-k^{2} \beta / 24\right)  \tag{Al}\\
G_{0}(k \mid \beta)= & \int_{0}^{0} D x \delta(\bar{x}-\xi)=\sqrt{12} l_{0}^{2} \exp \left(-6 \xi^{2} / \beta\right)  \tag{A2}\\
H_{0}(k \mid \beta)= & \int_{0}^{0} D x \exp [-i \lambda x(t)]=l_{0} \exp \left(-\frac{1}{2} \lambda^{2} \beta s\right)  \tag{A3}\\
I_{0}(\eta, t \mid \beta)= & \int_{0}^{0} D x \delta(x(t)-\eta)=l_{0}^{2} s^{-1 / 2} \exp \left(-\eta^{2} / 2 s\right)  \tag{A4}\\
J_{0}(k|\lambda, t| \beta)= & \int_{0}^{0} D x \exp [i k \bar{x}-i \lambda x(t)] \\
= & l_{0} \exp \left[-\left(k^{2} \beta / 24\right)-\left(\lambda^{2} \beta s / 2\right)+k \lambda \beta s / 2\right]  \tag{A5}\\
K_{0}(\xi|\lambda, t| \beta)= & \int_{0}^{0} D x \delta(\bar{x}-\xi) \exp [-i \lambda x(t)] \\
= & \sqrt{12} l_{0}^{2} \exp -\left[\frac{\lambda^{2} \beta s}{2}-\frac{6}{\beta}\left(\xi-i \frac{\lambda \sqrt{\beta}}{2} s\right)^{2}\right]  \tag{A6}\\
L_{0}(\xi|\eta, t| \beta)= & \int_{0}^{0} D x \delta(\bar{x}-\xi) \delta(x(t)-\eta) \\
= & \sqrt{12} l_{0}^{3}[s(1-3 s)]^{-1 / 2} \\
& \times \exp \left[-\frac{6 \xi}{\beta}-\frac{1}{2 \beta} \frac{(\eta+6 \xi s)^{2}}{s(1-3 s)}\right] \tag{A7}
\end{align*}
$$

$$
\begin{align*}
M_{0}(k|\eta, t| \beta) & =\int_{0}^{0} D x \delta(x(t)-\eta) \exp (i k \bar{x}) \\
& =l_{0}^{2} s^{-1 / 2} \exp \left[-\frac{k^{2}}{24}+\frac{1}{2} \beta s\left(\frac{k}{2}-\frac{i \eta}{\beta s}\right)^{2}\right] \tag{A8}
\end{align*}
$$

and

$$
\begin{align*}
& F\left(k|\beta|\left|x_{1} x_{2}\right|\right)= \int_{x(0)=x_{2}}^{x(\beta)=x_{1}} D x \exp (i k \bar{x}) \\
&= \exp \left[-k^{2} \beta / 24+i k\left(x_{1}+x_{2}\right) / 2\right] \rho_{0}\left(x_{1} x_{2} \mid \beta\right)  \tag{A9}\\
& G\left(\xi|\beta| \mid x_{1} x_{2}\right)= \sqrt{12} l_{0} \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \\
& \times \exp \left\{-(6 / \beta)\left[\xi-\left(x_{1}+x_{2}\right) / 2\right]^{2}\right\}  \tag{A10}\\
& H\left(\lambda, t|\beta| \mid x_{1} x_{2}\right)= \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \exp \left\{-\frac{1}{2} \lambda^{2} \beta s\right. \\
&\left.-i \lambda\left[x_{2}+(t \mid \beta)\left(x_{1}-x_{2}\right)\right]\right\}  \tag{A11}\\
& I\left(\eta, t|\beta| \mid x_{1} x_{2}\right)= l_{0} s^{-1 / 2} \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \\
& \times \exp \left\{-(1 / 2 \beta s)\left[\eta-x_{2}-(t \mid \beta)\left(x_{1}-x_{2}\right)\right]^{2}\right\}(\mathrm{A} 12)  \tag{A12}\\
& J\left(k|\lambda, t| \beta\left|\mid x_{1} x_{2}\right)=\right. \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \exp \left[-\frac{k^{2} \beta}{24}-\frac{\lambda^{2} \beta s}{2}+\frac{k \lambda \beta s}{2}\right] \\
& \times \exp \left\{i k \frac{x_{1}+x_{2}}{2}-i \lambda\left[x_{2}+\frac{t}{\beta}\left(x_{1}-x_{2}\right)\right]\right\}(\mathrm{A} 13)  \tag{A13}\\
& K\left(\xi|\lambda, t| \beta\left|\mid x_{1} x_{2}\right)=\right. \sqrt{12} l_{0} \rho_{0}\left(x_{1} x_{2} \mid \beta\right) \\
& \times \exp \left\{-\frac{\lambda^{2} \beta s}{2}-\frac{6}{\beta}\left[\xi-\frac{x_{1}+x_{2}}{2}-i \lambda \frac{\sqrt{\beta}}{2} s\right]^{2}\right\} \\
& \times \exp \left\{-i \lambda\left[x_{2}+\frac{t}{\beta}\left(x_{1}-x_{2}\right)\right]\right\}  \tag{A14}\\
& L\left(\xi|\eta, t| \beta\left|\mid x_{1} x_{2}\right)=\right. \sqrt{12} l_{0}^{2} \rho_{0}\left(x_{1} x_{2} \mid \beta\right)[s(1-3 s)]^{-1 / 2} \\
& \times \exp \left\{-(6 / \beta)\left[\xi-\frac{1}{2}\left(x_{1}+x_{2}\right)\right]^{2}\right\} \\
& \times \exp \left\{-\left[\eta-x_{2}-(t / \beta)\left(x_{1}-x_{2}\right)\right.\right. \\
&\left.\left.+6 s \xi-6 s\left(x_{1}+x_{2}\right) / 2\right]^{2}\{2 \beta s(1-3 s)]^{-1}\right\} \\
& \times \operatorname{La}\left(\xi-\frac{1}{2}\left(x_{1}+x_{2}\right)\left|\eta-x_{2}-(t / \beta)\left(x_{1}-x_{2}\right), t\right| \beta\right) \\
& M\left(k|\eta, t| \beta\left|\mid x_{1} x_{2}\right)=\right. M_{0}\left(k \mid \eta-\left(x_{1}-x_{2}\right)^{2} / 2 \beta\right]  \tag{A15}\\
& \text { (A15) }  \tag{Al6}\\
& \text { (A16) }
\end{align*}
$$

The average of the potential

$$
\begin{align*}
& \int_{0}^{0} D x \int_{0}^{\beta} V(x(t)) d t \\
& \quad=\int V(\eta) d \eta \int_{0}^{0} \beta x \int_{0}^{\beta} \delta(x(t)-\eta) d t \\
& \quad=\int V(\eta) d \eta \int_{0}^{\beta} I_{0}(\eta, t \mid \beta) d t=\int V(\eta) Q_{0}(\eta \mid \beta) d \eta \tag{A17}
\end{align*}
$$

with

$$
Q_{0}(\eta \mid \beta)=\frac{1}{2 \pi \beta} \int_{0}^{\beta} \frac{1}{\sqrt{s}} \exp \frac{-\eta^{2}}{2 \beta s} d t, \quad s=\frac{t}{\beta}\left(1-\frac{t}{\beta}\right)
$$

and

$$
\begin{align*}
& \int_{x}^{x_{1}} D x \int_{0}^{\beta} V(x(t)) d t=\int V(\eta) d \eta Q_{0}\left(\eta-x_{1} \mid \beta\right)  \tag{A18}\\
& \int_{x_{2}}^{x_{1}} D x \int_{0}^{\beta} V(x(t)) d t \\
& \quad=\int V(\eta) d \eta \int_{0}^{\beta} d t \int_{x_{2}}^{x_{1}} D x \delta(x(t)-\eta) \\
& \quad=\int V(\eta) d \eta \int_{0}^{\beta} d t I\left(\eta, t|\beta| \mid x_{1} x_{2}\right) Q\left(\eta|\beta| \mid x_{1} x_{2}\right) \tag{A19}
\end{align*}
$$

For the $\xi$-dependent part

$$
\begin{array}{rl}
\int_{0}^{0} D x & x(\bar{x}-\xi) \int_{0}^{\beta} V(x(t)) d t \\
= & \int V(\eta) d \eta \int_{0}^{\beta} d t L_{0}(\xi|\eta, t| \beta) \\
& \equiv \int V(\eta) d \eta R_{0}(\xi|\eta| \beta) \\
\int_{x_{1}}^{x_{1}} D x & \delta(\bar{x}-\xi) \int_{0}^{\beta} V(x(t)) d t \\
= & \int V(\eta) d \eta R_{0}\left(\xi-x_{1}\left|\eta-x_{1}\right| \beta\right) \\
\int_{x_{2}}^{x_{1}} D x \delta(\bar{x}-\xi) \int_{0}^{\beta} V(x(t)) d t \\
=\int V(\eta) d \eta R\left(\xi|\eta| \beta| | x_{1} x_{2}\right) \tag{A22}
\end{array}
$$

with

$$
R\left(\xi|\eta| \beta\left|\mid x_{1} x_{2}\right)=\int_{0}^{\beta} L\left(\xi|\eta, t| \beta| | x_{1} x_{2}\right) d t\right.
$$

## Path Integrals for the Harmonic Oscillator

$$
\begin{gather*}
\int_{x_{2}}^{x_{1}} D x \int_{0}^{\beta} \frac{x^{2}(t) d t}{2} D x \int_{0}^{\beta} \frac{x^{2}(t) d t}{2}=\frac{1}{(2 \pi \beta)^{1 / 2}} \frac{\beta^{2}}{12}  \tag{A23}\\
=\frac{1}{(2 \pi \beta)^{1 / 2}}\left\{\exp \left[-\frac{\left(x_{1}-x_{2}\right)^{2}}{2 \beta}\right]\right\} \frac{\beta^{2}}{12}\left[1+\frac{6 x_{1} x_{2}}{\beta}+\frac{2}{\beta}\left(x_{1}-x_{2}\right)^{2}\right] \\
 \tag{A24}\\
\int_{0}^{0} D x \delta(\bar{x}-\xi) \int_{0}^{\beta} \frac{x^{2}(t) d t}{2}=\frac{\sqrt{12}}{2 \pi} \beta\left(\frac{1}{30}+\frac{3}{5} \frac{\xi^{2}}{\beta}\right) \exp \frac{-6 \xi^{2}}{\beta}  \tag{A25}\\
\begin{aligned}
\int_{x_{1}}^{x_{1}} \begin{aligned}
D x & \delta(\bar{x}-\xi) \int_{0}^{\beta} \frac{x^{2}(t) d t}{2} \\
= & \frac{\sqrt{12}}{2 \pi} \beta\left[\frac{1}{30}+\frac{3}{5} \frac{\left(\xi-x_{1}\right)^{2}}{\beta}+\frac{1}{2} \frac{x_{1}{ }^{2}}{\beta}+\frac{x_{1}\left(\xi-x_{1}\right)}{\beta}\right] \exp \frac{-6\left(\xi-x_{1}\right)^{2}}{\beta} \\
& \int_{x_{2}}^{x_{1}} D x\left(\delta(\bar{x}-\xi) \int_{0}^{\beta} \frac{x^{2}(t) d t}{2}\right. \\
& \frac{\sqrt{12}}{2 \pi} \beta\left[\frac{1}{30}+\frac{3}{5 \beta}\left(\xi-\frac{x_{1}+x_{2}}{2}\right)\right. \\
& \left.+\frac{x_{1}+x_{2}}{2 \beta}\left(\xi-\frac{x_{1}+x_{2}}{2}\right)+\frac{x_{1} x_{2}}{2 \beta}+\frac{1}{6} \frac{\left(x_{1}-x_{2}\right)^{2}}{\beta}\right] \\
& \times \exp \left[-\frac{6}{\beta}\left(\xi-\frac{x_{1}+x_{2}}{2}\right)\right] \exp \left[-\frac{\left(x_{1}-x_{2}\right)^{2}}{2 \beta}\right]
\end{aligned}
\end{aligned}, \begin{array}{l}
\mathrm{A} 2
\end{array}
\end{gather*}
$$

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    ${ }^{1}$ Martin Fisher School of Physics, Brandeis University, Waltham, Massachusetts.

