Journal of Statistical Physics, Vol. 31, No. 1, 1983

Lower Bounds for Wiener Integrals

Eugene P. Gross[1]

Received October 11, 1982

Techniques are developed to sharpen lower bounds for density matrices occurring in statistical mechanics. The Wiener integrals are treated by insertion of trial functionals and parametric representations of unity that involve functionals of the path. Jensen's inequality is applied to suitable parameter-dependent path measures. These yield stronger forms than the basic Feynman bound. We also introduce trajectory insertions, and use coupling constant integration and the hierarchy for correlation functions to improve the bounds.

KEY WORDS: Density matrices; lower bounds; path integrals

1. INTRODUCTION

In the present paper we describe ways to improve lower bounds for Wiener integrals. In an earlier paper(1) we discussed two techniques to improve lower bounds for the density matrices that arise for a particle moving in a given potential. One is a time-slicing technique that is the basis of the construction of the Wiener integral. The main point was that time slicing leads to improved lower bounds. The second technique involves carrying out the integral in two stages. The first stage involves an integral for a fixed value of the mean position. In the second stage one integrates over all values of the mean position. This idea as applied to the partition function goes back to the book of Feynman and Hibbs.(2) It is a special case of a procedure called "reservation of variables" by Siegel and Burke.(3) Their emphasis was on systematic expansions, rather than on lower bounds.

In the present work we combine these ideas in a technique that involves insertion of representations of unity in the path integral. In Section

[1] Department of Physics, Brandeis University, Waltham, Massachusetts 02254.

2 we discuss insertions of the form

$$1 = \int \delta(z - F)\, dz\, e^{\beta} \cdot e^{-\beta} \tag{1}$$

where F and β are functionals of the path $x(u)$. Without loss of generality we may take $0 \leqslant u \leqslant 1$. The mean path position approach is a special case when $F = \bar{x} = \int_0^1 x\, du$. β is a trial functional. Lower bounds are obtained by applying the Jensen inequality[4] to the path integral. The key point is that the Wiener measure is replaced by a z-dependent measure. A further application of the Jensen inequality leads to the fundamental Feynman inequality. An interesting point is the connection of the insertion technique with the Feynman variation method. If $\beta = 0$, the insertion $1 = \int \delta(z - F)\, dz$ leads to the same results as the use of a trial functional $\omega(F)$ with the optimum choice of ω.

In Section 3 we discuss lower bounds obtained with insertions of the type

$$1 = \int \int \delta[x(t_1) - z_1]\delta[x(t_2) - z_2] \ldots dz_1 dz_2 \ldots \tag{2}$$

for some set $t_1, \ldots, t_n$. This is an economical way of introducing time slicing and can be used in conjunction with trial functionals β and insertions of the type discussed in Section 2. The technique is particularly useful for multitime path integrals.

In Section 4 we describe trajectory insertions, i.e., translations $x(u) \rightarrow x(u) + \xi(u)$, when $\xi(u)$ is a trajectory connecting the end points. While we do not pursue it here, it gives an idea of how semiclassical methods[5] can be improved by combining them with insertions and by using the lower bound property.

In Section 5 we introduce a coupling constant in the functional and use coupling constant integration to find bounds accurate to a given order in the coupling constant. We also outline how the hierarchy of correlation functions may be used to achieve the same end. Both of these methods involve finding bounds for correlation functions. This is again done by changing from Wiener measure to parameter-dependent singular measures.

Most of the methods described are not new and each one has undoubtedly been used in isolation in special problems. However, taken together from the general viewpoint of insertions, and anchored by the lower bound property, they combine to form a flexible instrument for the analysis of path integrals. In another paper[6] we generalized the Symanzik[7] idea to make a systematic study of upper bounds.

It goes without saying that our results are of a formal character, and there is no pretense at mathematical rigor.[8] All of our considerations have been developed for Wiener integrals, i.e., for density matrices. They can be made the basis of more systematic expansion procedures. We do not deal with this topic. It is a route that must be taken to deal with the complex Feynman integrals representing propagators.

2. THE INSERTION TECHNIQUE

Consider

$$\begin{aligned} \langle x_1 | I(t) | x_2 \rangle &= \int_{x_2}^{x_1} D_t x e^{A(t)} \\ D_t x &= \mathscr{D}_t x \exp\left(-\frac{1}{2} \int_0^t \dot{x}^2 \, du \right) \end{aligned} \tag{3}$$

i.e., Wiener measure. $A(t)$ is a functional of the path end $x(u)$, with end point parameter $u = t$. Since the limits x_1 and x_2 and the interval t will be almost always fixed we write frequently

$$\langle x_1 | I(t) | x_2 \rangle = E^* e^A \tag{4}$$

and read the parameters from the expression on the left-hand side. Note that

$$\int_{x_2}^{x_1} D_t x \equiv E^* 1 = \langle x_1 | \rho_0(1) | x_2 \rangle \tag{5}$$

is the free particle density matrix. All of our considerations are independent of the dimension of space.

Feynman's application of the Jensen inequality for the exponential function using Wiener measure (i.e., without a trial functional), gives

$$\langle x_1 | I(1) | x_2 \rangle \geqslant [E^* 1] \exp\left[\frac{E^* A}{E^* 1} \right] \tag{6}$$

With a trial functional β we write

$$\langle x_1 | I(1) | x_2 \rangle = \int_{x_2}^{x_1} D_1 x e^{\beta} e^{A - \beta} \tag{7}$$

Using a new measure

$$D_1 x e^{\beta} / E^* e^{\beta} \tag{8}$$

$$\langle x_1 | I(1) | x_2 \rangle \geqslant [E^* e^{\beta}] \exp\left[\frac{E^* (A - \beta) e^{\beta}}{E^* e^{\beta}} \right] \tag{9}$$

We strengthen this bound by a technique of insertion. Insert

$$1 = \int dz \, \delta(z - F) \tag{10}$$

where F is some functional. Interchange z and path integrations, and take as the (singular) measure for the path integration the z-dependent quantity

$$D_1 x\delta(z-F)/E^*\delta(z-F) \tag{11}$$

Jensen's inequality, applied for each z, gives

$$\langle x_1|I(1)|x_2\rangle \geqslant \int dz\left[E^*\delta(z-F)\right]\cdot\exp\left[\frac{E^*A\delta(z-F)}{E^*\delta(z-F)}\right] \tag{12}$$

if one adapts

$$E^*\delta(z-F)/E^*1 \tag{13}$$

as a weight for the z integration and applies the Jensen inequality again, one finds the simple Feynman bound. Thus, the insertion leads to a stronger inequality than the Feynman bound without a trial functional, for any F that leads to a finite result.

We may insert $e^{\beta}\cdot e^{-\beta}=1$. For each z take

$$D_1 x\delta(z-F)e^{\beta}/E^*\delta(z-F)e^{\beta} \tag{14}$$

as the singular measure for the path integration. Then

$$\langle x_1|I(1)|x_2\rangle \geqslant \int dz\left[E^*\delta(z-F)e^{\beta}\right]\exp\left[\frac{E^*\delta(z-F)e^{\beta}(A-\beta)}{E^*\delta(z-F)e^{\beta}}\right] \tag{15}$$

if we take as a weight for the z integration the expression

$$\frac{E^*\delta(z-F)e^{\beta}}{E^*e^{\beta}} \tag{16}$$

Jensen's inequality gives the Feynman bound with trial functional β.

We can relate this to familiar things by taking $F=\bar{x}$, $\bar{x}=\int_0^1 x(u)\,du$, in the inequality (12). With $\beta=0$ it becomes the mean path lower bound suggested by Feynman and Hibbs for the partition function. This was applied to the density matrix by Siegel and Burke,[3] Bruch and Revercomb,[9] and the author.[1] For any A we have

$$\langle x_1|I(1)|x_2\rangle \geqslant \int dz\left[E^*\delta(\bar{x}-z)\right]\exp\left[\frac{E^*\delta(\bar{x}-z)A}{E^*\delta(\bar{x}-z)}\right] \tag{17}$$

The path integrals can be evaluated by using the integral representation of the delta function

$$E^*\delta(z-\bar{x})=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{-i\alpha z}E^*e^{i\alpha\bar{x}}\,d\alpha \tag{18}$$

For the one-dimensional case

$$\int_{x_2}^{x_1}D_1 x\delta(\bar{x}-z)=\frac{\sqrt{12}}{(2\pi)^{1/2}}\langle x_1|\rho_0(1)|x_2\rangle\exp\left[-6\left(z-\frac{x_1+x_2}{2}\right)^2\right] \tag{19}$$

For a time-independent potential A has the form

$$A = \int d\eta\, \phi(\eta) \int_0^1 \delta[x(t) - \eta]\, dt \tag{20}$$

So we need $E^* \delta(\bar{x} - z)\delta[x(t) - \eta]$. This is given in (A15) of Ref. 1. The result is (in one dimension)

$$\int_{x_2}^{x_1} D_1 x \delta(\bar{x} - z)\delta[x(t) - \eta] = \frac{(12)^{1/2}}{2\pi} \frac{\langle x_1|\rho_0(1)|x_2\rangle}{[\sigma(1-3\sigma)]^{1/2}}$$
$$\times \exp\left\{ -6\left[z - \frac{(x_1 + x_2)}{2} \right]^2 \right\} \exp[-Q] \tag{21}$$

with

$$\sigma = t(1-t)$$
$$Q = \{\eta - x_2 - t[x_1 - x_2 + 6\sigma z - 3\sigma(x_1 + x_2)]\}^2 / 2\sigma(1-3\sigma)$$

For a "two-time" functional for A we need correlation functions of the type $E^*\delta(\bar{x} - z)\delta[x(t) - \eta]\delta[x(t_1) - \eta_1]$. These can be evaluated explicitly by the same technique.

There is an interesting relation between the insertion technique and the usual variational approach. If, in Feynman's inequality, we set $\beta = \omega(F)$, we find

$$\langle x_1|I(1)|x_2\rangle \geqslant \{E^* e^{\omega(F)}\} \exp\left\{ \frac{E^*[A - \omega(F)]e^{\omega(F)}}{E^* e^{\omega(F)}} \right\} \tag{22}$$

We can use a parametric representation for each factor. Thus

$$E^* e^{\omega(F)} = \int dz\, e^{\omega(z)} E^* \delta(z - F) \tag{23}$$

The function $\omega(z)$ can then be varied to find the best lower bound. This turns out to be equivalent to canceling the argument of the exponential. One finds

$$\begin{aligned} \omega(z) &= [E^*\delta(z-F)A]/[E^*\delta(z-F)] \\ \langle x_1|I(1)|x_2\rangle &\geqslant \int dz\, d^{\omega(z)} E^* \delta(z - F) \end{aligned} \tag{24}$$

This is the result of the insertion technique.

It is clear that this result is easily generalized. Given two functionals F_1 and F_2 (for example, $F_1 = \bar{x}$, $F_2 = \bar{x}^2$) one can look for optimum $\omega(F_1, F_2)$

in the standard bound. The result is the insertion bound

$$\begin{aligned} \langle x_1|I(1)|x_2\rangle &\geqslant \int dz_1 \int dz_2 \left[E^*\delta(z_1 - F_1)\delta(z_2 - F_2) \right] e^{\omega(z_1, z_2)} \\ \omega(z_1, z_2) &= \left[E^* A\delta(z_1 - F_1)\delta(z_2 - F_2) \right] / E^*\delta(z_1 - F_1)\delta(z_2 - F_2) \right] \end{aligned} \tag{25}$$

A standard approach to many time functionals A is to use a potential type trial functional

$$\beta = \int_0^1 \psi[x(u)]\, du \tag{26}$$

in the Feynman bound. One needs the density matrix

$$\langle x_1|\rho_\psi(T)|x_2\rangle = \int_{x_2}^{x_1} D_T x \exp\left\{ \int_0^T \psi[x(u)]\, du \right\} \tag{27}$$

It can be computed by path integral methods or from the Bloch differential equation via the Kac relation.[10] The correlation functions can be computed from the Markov property:

$$\langle x_1|\rho_\psi(T)|x_2\rangle = \int \langle x_1|\rho_\psi(T - t)|z\rangle\, dz\, \langle z|\rho_\psi(t)|x_2\rangle \tag{28}$$

The improved bound involves $\omega\{\int_0^1 \psi[x(u)]\, du\}$ and can be computed using

$$E^*\delta\left\{ z - \int_0^1 \psi[x(u)]\, du \right\} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\alpha\, e^{-i\alpha z} E^* e^{i\alpha \int_0^1 \psi[x(u)]\, du} \tag{29}$$

Thus we need the density matrix for a variable, imaginary strength.

Another example occurs in the analysis of two time functionals A. One common approach is to use a quadratic trial functional $F_1 + F_2$ with

$$\begin{aligned} F_1 &= \int_0^1 \int_0^1 x(u)\Lambda(u \mid u')x(u')\, du\, du' \\ F_2 &= \int_0^1 \lambda(u)x(u)\, du \end{aligned} \tag{30}$$

The Gaussian integrals can be done explicitly. Again, the insertion technique generalizes this to an optimum $\omega(F_1, F_2)$.

We note finally that one could compute a variational bound with a less than optimal $\omega_0(F)$. This follows from the bound obtained with the insertion $1 = \int dz\, \delta(z - F)$. One inserts $e^{\omega_0(z)} \cdot e^{-\omega_0(z)}$ and takes

$$\frac{E^*\delta(z - F)e^{\omega_0(z)}}{E^* e^{\omega_0(F)}} \tag{31}$$

as a weight for the z integration. Then one applies Jensen's inequality.

3. CORRELATION INSERTIONS

Consider the insertion

$$1 = \int_0^1 \delta[x(t) - z]\,dz, \qquad 0 < t < 1 \tag{32}$$

Use a trial functional β. The singular measure for path integration is

$$\{D_1 x\delta[x(t) - z]e^{\beta}\}/\{E^*\delta[x(t) - z]e^{\beta}\} \tag{33}$$

This depends on z and t as well as the end points x_1, x_2. We have the bound

$$\langle x_1|I(1)|x_2\rangle \geqslant \int dz\,\{E^*\delta[x(t) - z]e^{\beta}\}\exp\left\{\frac{E^*(A-\beta)e^{\beta}\delta[x(t) - z]}{E^*\delta[x(t) - z]e^{\beta}}\right\} \tag{34}$$

One expects that there will be a $t = t^*$ that optimizes the bound. We will not be concerned with this. Instead, consider some weakening of the bound, that still leaves us with results stronger than the elementary Feynman bound. Note that, for any t, the application of Jensen's inequality to the z integration with weight

$$\{E^*\delta[x(t) - z]e^{\beta}\}/[E^*e^{\beta}] \tag{35}$$

yields Feynman's result.

It is more interesting to integrate with respect to t. For fixed z, use

$$\begin{gathered} dt\{E^*\delta[x(t) - z]e^{\beta}\}/[E^*c(z)e^{\beta}] \\ c(z) = \int_0^1 \delta[x(u) - z]\,du \end{gathered} \tag{36}$$

as the measure for the t integration. Then

$$\langle x_1|I(1)|x_2\rangle \geqslant \int dz\,[E^*c(z)e^{\beta}]\exp\left[\frac{E^*c(z)e^{\beta}(A-\beta)}{E^*c(z)e^{\beta}}\right] \tag{37}$$

This can be obtained by the insertion $1 = \int c(z)\,dz$.

The obvious generalization is obtained by inserting

$$1 = \int \cdots \int dz_1 \cdots dz_n \delta\{[x(t_1) - z_1] \cdots \delta[x(t_n - z_n)]\} \tag{38}$$

It is

$$\langle x_1|I(1)|x_2\rangle \geqslant \int\int dz_1 \cdots dz_n \left\{E^*\delta[x(t_1)-z_1]\cdots\delta[x(t_n)-z_n]e^{\beta}\right\}$$
$$\times \exp\left\{\frac{E^*(A-\beta)e^{\beta}\delta[x(t_1)-z_1]\cdots\delta[x(t_n)-z_n]}{E^*\delta[x(t_1)-z_1]\cdots\delta[x(t_n)-z_n]e^{\beta}}\right\} \tag{39}$$

The insertions of the previous section may be combined with those discussed here.

To relate to familiar results, we examine the single time

$$A=\int_0^1 \phi[x(u)]\,du \tag{40}$$

We have the Markov property

$$\langle x_1|I(1)|x_2\rangle \int dz\,\langle x_1|I(1-t)|z\rangle\langle z|I(t)|x_2\rangle, \qquad 0<t<1 \tag{41}$$

We study only the case where there is no trial functional. The simple Feynman bound for the unit interval is

$$\langle x_1|I(1)|x_2\rangle \geqslant \langle x_1|\rho_0(1)|x_2\rangle$$
$$\times \exp\left[\frac{\int d\eta \int_0^1\langle x_1|\rho_0(1-u)|\eta\rangle\langle\eta|\rho_0(u)|x_2\rangle\phi(\eta)\,du}{\langle x_1|\rho_0(1)|x_2\rangle}\right] \tag{42}$$

On the other hand, accepting the Markov property, one may bound the two factors separately. This leads to

$$\langle x_1|I(1)|x_2\rangle \geqslant \int dz\,\langle x_1|\rho_0(1-t)|z\rangle\langle z|\rho_0(t)|x_2\rangle \exp\left[\int\phi(\eta)P(\eta)\,d\eta\right] \tag{43}$$

with

$$P(\eta)=\int_t^1 du\,\langle x_1|\rho_0(1-u)|\eta\rangle\langle\eta|\rho_0(u)|z\rangle$$
$$+\int_0^t du\,\langle z|\rho_0(t-u)|\eta\rangle\langle\eta|\rho_0(u)|x_2\rangle \tag{44}$$

This "time-slicing" procedure improves the bound. We recover the bound given by Eq. (42) by applying the Jensen inequality to the z integration with

$$\langle x_1|\rho_0(1-t)|z\rangle\langle z|\rho_0(t)|x_2\rangle/\langle x_1|\rho_0(1)|x_2\rangle \tag{45}$$

as a weight.

It may be checked that the insertion $1=\int\delta[x(t)-z]\,dz$ gives the same result as the time-slicing procedure for the potential case. The insertion $1 = \int c(z)\,dz$ gives a time-averaged bound.

Correlation insertions are more interesting for a two time A of the form

$$
\begin{aligned}
A &= \frac{1}{2}\int_0^1\int_0^1 du_1\,du_2\,W[x(u_1) - x(u_2)] \\
&= \frac{1}{2}\int\int d\eta\,d\eta_1\,W(\eta - \eta_1)c(\eta)c(\eta_1)
\end{aligned}
\tag{46}
$$

The elementary Feynman bound without trial action is

$$
\begin{aligned}
\langle x_1|I(1)|x_2\rangle \geqslant \langle x_1|\rho_0(1)|x_2\rangle \exp\Bigg[\frac{1}{2\langle x_1|\rho_0(1)|x_2\rangle}\int\int W(\eta_1 - \eta_2)\,d\eta_1\,d\eta_2 \\
\times E^* c(\eta_1)c(\eta_2)\Bigg]
\end{aligned}
\tag{47}
$$

$c(\eta_1)$ and $c(\eta_2)$ can be split into contributions from 0 to t and from t to 1. We no longer have the Markov property. $E^*c(\eta_1)c(\eta_2)$ then has two contributions from the same time intervals and two crossed terms. The term involving both 0 to t intervals is

$$
\int\int d\eta_1\,d\eta_2 \int_{x_2}^{x_1} D_t x \int_0^t \delta[x(u_1) - \eta_1]\,du_1 \cdot \int_0^t \delta[x(u_2) - \eta_2]\,du_2 \cdot \tfrac{1}{2} W(\eta_1 - \eta_2)
\tag{48}
$$

It has the value

$$
\begin{aligned}
\int\int d\eta_1\,d\eta_2\,W(\eta_1 - \eta_2)\int_0^t du_1 \int_0^{u_1} du_2 \langle x_1|\rho_0(t - u_1)|\eta_1\rangle\langle \eta_1|\rho_0(u_1 - u_2)|\eta_2\rangle \\
\times \langle \eta_2|\rho_0(u_1)|x_2\rangle
\end{aligned}
\tag{49}
$$

This type of term involves three free particle density matrices. There is a similar contribution from the interval t to 1. The contribution of the crossed terms involves four free particle density matrices. It is

$$
\begin{aligned}
\int d\eta \int\int W(\eta_1 - \eta_2)\,d\eta_1\,d\eta_2 \int_t^1 \langle x_1|\rho_0(1 - u)|\eta_1\rangle\langle \eta_1|\rho_0(u - t)|\eta\rangle\,du \\
\times \int_0^t \langle \eta|\rho_0(t - u_2)|\eta_2\rangle\langle \eta_2|\rho_0(u_2)|x_2\rangle\,du_2
\end{aligned}
\tag{50}
$$

Contrast this with the insertion $1 = \int \delta(t) - \eta)\,d\eta$, which is an economical way of performing time splitting. We have Eq. (34) with $\beta = 0$. Again the term involving A has several types of contributions. The difference between the two types of bounds is already evident with the weaker insertion $1 = \int c(\eta)\,d\eta$. Then

$$\langle x_1|I(1)|x_2\rangle \geqslant \int d\eta\left[E^*c(\eta)\right] \cdot \exp\left[\frac{\frac{1}{2}\iint W(\eta_1-\eta_2)E^*c(\eta)c(\eta_1)c(\eta_2)\,d\eta_1\,d\eta_2}{E^*c(\eta)}\right] \tag{51}$$

This involves higher-order correlation functions. The insertion

$$1 = \int\int\int \delta\left[x(t)-z\right]\delta\left[\frac{1}{t}\int_0^t x(u)\,du - z_1\right] \times \delta\left[\frac{1}{1-t}\int_t x(u)\,du - z\right]dz\,dz_1\,dz_2 \tag{52}$$

divides the interval into two pieces and holds the mean positions of the segments at positions z_1 and z_2. Approximations made on the conditional path integral give effective interactions between the segment's mean positions.

4. INTRODUCTION OF A TRAJECTORY

Consider first the single time $A = \int_0^1 \phi[x(u)]\,du$. Let $\xi(u)$ be a "trajectory" such that $\xi(0) = x_2$, $\xi(1) = x_1$, and make the translation in function space:

$$x(u) = \xi(u) + y(u) \tag{53}$$

This yields (after an integration by parts with $y(0) = y(1) = 0$),

$$\langle x_1|I(1)|x_2\rangle = \exp\left(-\tfrac{1}{2}\int_0^1 \dot{\xi}^2\,du\right)\int_0^0 D_1 y \exp\left[\int_0^1 \ddot{\xi}(u)y(u)\,du\right] \times \exp\left\{\int_0^1 \phi\left[\xi(u)+y(u)\right]du\right\} \tag{54}$$

For a two-time action

$$A \to \tfrac{1}{2}\int_0^1\int_0^1 W\left[\xi(u)-\xi(u')+y(u)-y(u')\right]du\,du' \tag{55}$$

The lower-bound techniques may be applied for any suitable $\xi(u)$ and we may then set about finding the optimum $\xi(u)$. Thus the elementary Feynman bound without trial functional yields for the potential problem

$$\langle x_1|I(1)|x_2\rangle \geqslant \exp\left(-\tfrac{1}{2}\int \dot{\xi}\,du\right)\langle 0|\rho_0(1)|0\rangle \times \exp\frac{\left\{dz\int_0^1\phi\left[\xi(u)+z\right]\int_Q^0 D_1 x\delta\left[y(u)-z\right]du\,dz\right\}}{\langle 0|\rho_0(1)|0\rangle}$$

$$\int_0^0 D_1 x\delta\left[y(u)-z\right]\rangle = \langle 0|\rho_0(1-u)|z\rangle\langle z|\rho_0(u)|0\rangle \tag{56}$$

This is a useful form for obtaining lower bounds on the behavior of I as a function of x_1 and x_2. For example, we obtain a simple, explicit bound with the straight line choice

$$\xi(u) = x_2 + u(x_1 - x_2)$$
$$\tfrac{1}{2}\int_0^1 \dot{\xi}^2\,du = \frac{(x_2 - x_1)^2}{2} \tag{57}$$

To make contact with semiclassical theory, write

$$\begin{aligned}\int_0^1 \phi[\xi(u) + y(u)]\,du = \int_0^1 \phi[\xi(u)]\,du + \int_0^1 y(u)\phi'[\xi(u)]\,du \\ + \int_0^1 \{\phi[\xi(u) + y(u)]\,du - \phi[\xi(u)] \\ - y(u)\phi'[\xi(u)]\,du\}\end{aligned}$$

We see if there are solutions of

$$\ddot{\xi}(u) + \phi'[\xi(u)] = 0, \qquad \xi(0) = x_2, \quad \xi(1) = x_1 \tag{59}$$

One can then bound the density matrix by the Feynman inequality with no trial action. The next step is to examine the quadratic term in the expansion, viz.

$$\frac{1}{2!}\int_0^1 \psi''[\xi(u)]\,y^2(u)\,du \tag{60}$$

If $\phi''[\xi(u)] < 0$ everywhere on the trajectory (as in the much discussed[5] quartic oscillator $\phi = \lambda\xi^4/4$, $\lambda > 0$), there is no difficulty. One can absorb the quadratic term into a trial action and proceed with the Laplace method. However, a simple potential such as $\phi(\xi) = g\exp(-\xi^2/b^2)$ has continuum eigenfunctions and possibly bound states. The curvature $\phi''(\xi)$ can be either positive or negative, depending on the end points x_1 and x_2. It is not sensible to include the quadratic terms on the trial functional for the regions $\phi''(\xi) > 0$ in this type of treatment. We have not made a serious study of this problem. But the technique of insertions should help. For example, suppose one starts at a point x_2 where $\phi''(x_2) < 0$. Insert $1 = \int\delta[x(y) - z]\,dz$ for some small value of t. For the points z where $\phi''[\xi(u)]$ $(0 < u < t)$ is negative we proceed with the Laplace expansion. A crude approach is then to use the free action bounds for all other values of z. Of course, a better approximation would be to make further insertions to treat the parts of the trajectories from x_2 to those z where $\phi'' < 0$.

5. COUPLING CONSTANT INTEGRATION AND THE HIERARCHY

There is an elementary way of improving bounds. Start with the identity

$$e^{gA} - 1 = \int_0^g dg_1 \frac{\partial}{\partial g_1}(e^{g_1 A}) = \int_0^g dg_1 A e^{g_1 A} \tag{61}$$

Repeating this

$$e^{gA} - 1 = gA + \int_0^g dg_1 (g - g_1) A^2 e^{g_1 A} \tag{62}$$

We then find

$$\langle x_1 | I_g(1) - \rho_0(1) | x_2 \rangle = \int_0^g dg_1 E^* A e^{g_1 A} \tag{63}$$

$$\langle x_1 | I_g(1) - \rho_0(1) | x_2 \rangle = gE^* A + \int_0^1 dg_1 (g - g_1) E^* A^2 e^{g_1 A} \tag{64}$$

We now need bounds for the correlation functions occurring on the right-hand side. The first equation is most useful when A has a definite sign for all paths. If $A > 0$ lower bounds remain lower bounds, while if $A < 0$ upper and lower bounds for $E^*|A|e^{g_1 A}$ on the right-hand side are converted to lower and upper bounds for the density matrix. The second equation preserves lower bounds and can be used even if A does not have a definite sign.

We have already noted the utility of coupling constant integration in connection with the method of obtaining upper bounds using the Symanzik technique. Here we apply the identities to the lower-bound problem.

Consider first the case where there is no trial functional and A is > 0. Use

$$D_1 x A \Big/ \int_{x_2}^{x_1} D_1 x A \tag{65}$$

as a path measure. Using the first identity and defining

$$\langle x_1 | J_g(1) | x_2 \rangle \equiv \int_{x_2}^{x_1} D_1 x A e^{gA} \tag{66}$$

we have

$$\langle x_1 | J_g(1) | x_2 \rangle \geqslant [E^* A] \exp\left[g \frac{E^* A^2}{E^* A} \right] \tag{67}$$

$$\langle x_1 | I_g(1) - \rho_0(1) | x_2 \rangle \geqslant \frac{[E^* A]^2}{[E^* A^2]} \left\{ \exp\left[g \frac{E^* A^2}{E^* A} \right] - 1 \right\} \tag{68}$$

The result is accurate to order g^2. With a trial action $\beta(g)$ the same method yields

$$\langle x_1|J_g(1)|x_2\rangle \geqslant [E^*Ae^{\beta(g)}]\exp\left[\frac{E^*A(gA-\beta)e^{\beta}}{E^*e^{\beta}A}\right] \tag{69}$$

The second identity requires the evaluation of

$$\langle x_1|K_g(1)|x_2\rangle \equiv E^*A^2e^{gA} \tag{70}$$

The lower bound is

$$\langle x_1|K_g(1)|x_2\rangle \geqslant [E^*A^2e^{\beta}]\exp\left[\frac{E^*(gA-\beta)A^2e^{\beta}}{E^*A^2e^{\beta}}\right] \tag{71}$$

This leads to a lower bound accurate to order g^3 for I_g.

The coupling constant integration is useful when one has a way of evaluating J_g or K_g for large values of g that is not accurate for $g < 1$. In that region more conventional methods can be used.

Stronger bounds for J_g or K_g are available. We only treat the case where A has a definite sign. These depend on the form of A. When A has the form appropriate for a potential

$$\begin{aligned}\langle x_1|K_g(1)|x_2\rangle &\geqslant \int\int \phi(\eta_1)\phi(\eta_2)\,d\eta_1\,d\eta_2\left\{E^*\delta[x(t_1)-\eta_1]\delta[x(t_2)-\eta_2]e^{\beta}\right\}\\ &\quad\times\exp\left\{\frac{E^*\delta[x(t_1)-\eta_1]\delta[x(t_2)-\eta_2](gA-\beta)e^{\beta}}{E^*\delta[x(t_1)-\eta_1]g[x(t_2)-\eta_2]e^{\beta}}\right\}\end{aligned} \tag{72}$$

provided $\phi(\eta)$ has the same sign for all η. Of course, one can make additional insertions.

For a two-time action the strongest form, without insertions, for $W \geqslant 0$ is

$$\begin{aligned}\langle x_1|J_g(1)|x_2\rangle &\geqslant \tfrac{1}{2}\int\int W(\eta_1-\eta_2)\,d\eta_1\,d\eta_2\int_0^1 dt_1\int_0^1 dt_2\\ &\quad\times\left[E^*\delta[x(t_1)-\eta_1]\delta[x(t_2)-\eta_2]e^{\beta}\right]\\ &\quad\times\exp\left\{\frac{E^*(A-\beta)e^{\beta}\delta[x(t_1)-\eta_1]\delta[x(t_2)-\eta_2]}{E^*\delta[x(t_1)-\eta_1]\delta[x(t_2)-\eta_2]e^{\beta}}\right\}\end{aligned} \tag{73}$$

Finally, as in our paper on upper bounds, we note that the hierarchy of correlation functions can be used to improve bounds. For potential functions

$$\langle x_1|I_g(T)-\rho_0(T)|x_2\rangle = g\int dz\int_0^T\langle x_1|\rho_0(T-t)|z\rangle\langle z|I_g(t)|x_2\rangle\,dt\,\phi(z) \tag{74}$$

For $\phi(z) \geqslant 0$ we increase the accuracy by bounding $\langle z|I_g(t)|x_2\rangle$. If $\phi(z) \leqslant 0$ we iterate the above equation once.

For a two-time action the first equation in the hierarchy is

$$\langle x_1|I(T) - \rho_0(T)|x_2\rangle = \int\int \langle x_1|\rho_0(T - t)|z\rangle \, dz \, W(y - z) \, dy \times \int_{x_2}^{z} D_t x \int_0^t \delta[x(u) - y] e^{A(t)} \, du \tag{75}$$

For $W > 0$ it suffices to bound the correlation function by the techniques already described.

REFERENCES

1. E. P. Gross, *J. Stat. Phys.* **21**:215 (1979).
2. R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965); R. P. Feynman, *Statistical Mechanics* (W. A. Benjamin Inc., Reading, Massachusetts, 1972).
3. A. Siegel and T. Burke, *J. Math. Phys.* **13**:1681 (1972); *Adv. Chem. Phys.* **15**:355 (1969).
4. G. H. Hardy, J. E. Littlewood, and G. Polya, *Inequalities*, 2nd ed., (Cambridge University Press, Cambridge, England, 1967).
5. M. M. Mizrachi, *J. Math. Phys.* **20**(5):844 (1979); **19**:298 (1978); **17**:566 (1976).
6. E. P. Gross, *J. Stat. Phys.*, in press.
7. K. Symanzik, *J. Math. Phys.* **6**:1155 (1965).
8. B. Simon, *Functional Integration and Quantum Physics* (Academic Press, New York, 1979); C. DeWitt-Morette, A. Maheshwari, and B. Nelson, *Phys. Reports*, No. 5:255 (1979); L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley–Interscience, New York, 1981).
9. L. W. Bruch and H. E. Revercomb, *J. Chem. Phys.* **58**:751 (1973).
10. M. Kac, *Probability and Related Topics on the Physical Sciences* (Interscience, New York, 1959).