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Upper Bounds for Density Matrices Using Path Integrals

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We discuss upper bounds for density matrices for a particle, that occur in potential theory, and as a result of averaging over other degrees of freedom. The Weiner path integral representation is used. A basic technique of Symanzik is generalized in a variety of ways to a series of sharper upper bounds. There are distinct ways of applying the technique to the two-parameter integrals that describe averaged density matrices. A single-parameter application of the Symanzik technique leads to a temperature-dependent potential problem. The nature of the bounds is illustrated for two-parameter integrals by studying a soluble quadratic action, a one-dimensional delta correlation function action and shell correlation functions. The dependence on dimension is studied in the latter case.

KEY WORDS: Upper bounds; path integrals; density matrices.

1. INTRODUCTION

The present paper treats the problem of finding upper bounds (UB) for density matrices. We use the path (Wiener) integral representation. The integers are of the form

$$\langle x_1|I(\beta)|x_2\rangle = \int_{x_2}^{x_1} D_\beta x \exp[A(\beta)] \tag{1}$$

Here,

$$D_\beta x = \mathfrak{D}_\beta x \exp\left[-\frac{1}{2}\int_{x_2}^{x_1}\left(\frac{dx}{du}\right)^2 du\right] \tag{2}$$

i.e., we use Wiener measure.

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For a particle subject to a time-dependent potential, $-\phi(x \mid t)$, we have

$$A(\beta) = \int_0^{\beta} \phi(x(u), u)\, du \tag{3}$$

we refer to u as the "time" variable and to $A(\beta)$ as the "action." For a free particle the action is zero.

Our main interest is in the study of "two-time" actions, when $A(\beta)$ has the form

$$A(\beta) = \frac{1}{2} \int_0^{\beta} \int_0^{\beta} W\left[x(u) - x(u') \,\|\, u - u'\right] du\, du' \tag{4}$$

This type of action arises in the problem of a particle subject to random potentials, after one performs the average over a Gaussian distribution. $W(x)$ is the time-independent correlation function and is positive and short range in the simplest situation. An explicitly time-dependent, positive, $W(x \,\|\, u)$ appears in the path integral formulation of large polaron theory. The case where $W(x) < 0$ appears in the continuum formulation of the excluded volume polymer problem. There, β is the length of the chain and $\mathbf{x}(u)$ is the position of a point that is u units along the chain.

Our analysis consists of elaborations, generalizations, and applications of a key idea due to Symanzik.[1] Most of the results apply to explicitly time-dependent actions. However, to keep things simple, we restrict ourselves to the time-independent case. Symanzik's approach has been discussed by Bruch and Revercomb,[2] Lieb,[3] and Simon.[4]

In Section 2 we review the application to potential theory. There are two types of UB, referred to as the weaker and stronger bounds. For both of these we introduce a set of sharper bounds that are denoted as multipoint or N-point bounds. As $N \to \infty$ the bounds approach the exact result. However, none of the bounds are accurate to order ϕ^2. We show how to use the integral equation obeyed by $I(s)$ to achieve this. In addition we comment on the use of trial actions to improve the bounds.

In Section 3 we apply Symanzik's technique to double time bounds, where both u and u' variables are subjected to the Jensen inequality. These bounds and their multipoint generalizations are rather weak. For example they are infinite when $W(x)$ is a one-dimensional delta function. They feature correlation functions for the free action.

In Section 4, we study single time UB, based on treating only one of the time variables by the Symanzik technique. The results are much more interesting. First we treat the action symmetrically in the time variables. The UB are determined by a β-dependent potential $\phi(x) = \beta W(x)/2$. Second, we show that there is an alternative, asymmetric decomposition. Here the UB involves a potential with twice the strength, viz., $\phi(x)$

$= \beta W(x)$. For $W(x) > 0$ the symmetric bound is shown to be sharper. For both types of bounds we derive the N-point improvements.

In Section 5 we consider the problem of obtaining bounds that are accurate to order W^2. This is done with the hierarchy that links correlation functions. One needs bounds for the correlation functions. These are obtained easily, but the results are complicated.

In Section 6 the nature of the results is illuminated by comparison with the exact answers for a soluble two time quadratic action. A brief comparison is made with the corresponding lower bounds obtained by using a single time harmonic trial action.

Section 7 is concerned with the one-dimensional delta function correlation function (white noise) $W(x) = V_0\delta(x)$. For $\beta \gg 1$, the symmetrical UB has a dominant exponential involving a term proportional to $V_0^2\beta^3$. This comes from the single bound state. However, the coefficient is three times larger than the exact result. For $\beta \ll 1$ the long spatial tail due to the bound state is washed out by interference from the distorted continuum states.

In Section 8 we examine shell potentials located at unit distance from the origin. For $V_0\beta \gg 1$ the results for all dimensions are similar to those for one-dimensional delta function. For $V_0\beta \ll 1$ the weak bound state in two dimensions leads to nonanalytic contributions, not recoverable from the perturbation series. We note that for $\beta \gg 1$ the partition function has a different dependence for shell correlation functions than it does for potential hole or smooth correlations. The shell functions behave like the one-dimensional delta function, with an exponential dependence on $V_0^2\beta^3$. For the less singular correlation functions, the dominant exponential is proportional to $V_0\beta$. The bound states have eigenvalues with a leading term proportional to the strength of the potential.

2. POTENTIAL THEORY

First we consider bounds involving the free action. Let

$$A(s) = \int_0^s \phi(x(u))\, du \tag{5}$$

We need the free particle density matrix in ϵ dimensions

$$\langle x_1|\rho_0(s)|x_2\rangle = \int_{x_2}^{x_1} D_s x = (2\pi s)^{-\epsilon/2}\exp\left[\frac{-(\mathbf{x}_2-\mathbf{x}_1)^2}{2s}\right] \tag{6}$$

Let

$$\Delta_s x = \frac{D_s x}{\langle x_1|\rho_0(s)|x_2\rangle} \tag{7}$$

so that

$$\int_{x_2}^{x_1} \Delta_s x = 1 \tag{7'}$$

Feynman's lower bound[5] is based on Jensen's equality when applied to $\Delta_s x$. It is

$$\langle x_1 | I(s) | x_2 \rangle \geqslant \langle x_1 | \rho_0(s) | x_2 \rangle \exp\left[\int_{x_2}^{x_1} \Delta_s x A(s) \right] \tag{8}$$

the operation $\int_{x_2}^{x_1} D_s x$ applied to a functional occurs so frequently that we use the notation

$$\langle x_1 | I(s) | x_2 \rangle \equiv \int_{x_2}^{x_1} D_s x F(s) \rightarrow E^* F(s) \tag{9}$$

Here, the end points of the integration and the range of the E^* operation can be read in the quantity on the left-hand side.

Symanzik's weaker UB is based on an application of Jensen's inequality to the u integration (with weight $1/s$). Since $I(s)$ has the u integration in the exponential, one gets an UB:

$$\frac{1}{s} \int_0^s du \exp[s\phi(x(u))] \geqslant \exp[A(s)] \tag{10}$$

$$\langle x_1 | I(s) | x_2 \rangle \leqslant E^* \int_0^s \frac{du}{s} \exp[s\phi(x(u))] \tag{11}$$

To obtain an explicit result, insert, for each u

$$1 = \int \delta(x(u) - z)\, dz \tag{12}$$

$$\begin{aligned} \langle x_1 | I(s) | x_2 \rangle &\leqslant E^* \int_0^s \frac{du}{s} \int dz\, \delta(x(u) - z) \exp[s\phi(z)] \\ &\leqslant \int_0^s \frac{du}{s} \int \langle x_1 | \rho_0(s-u) | z \rangle \exp[s\phi(z)] \langle z | \rho_0(u) | x_2 \rangle\, dz \end{aligned} \tag{13}$$

One finds the Golden–Thompson[6] bound for the partition functions

$$Z(s) = \int dx_1 \langle x_1 | I(s) | x_1 \rangle \leqslant \int dz \exp[s\phi(z)] \tag{14}$$

A much stronger bound for the partition function has been obtained by Barnes, Brascamp, and Lieb[7] for potentials that have all discrete status. We are, however, interested in functions $\phi(z)$ that are short range, such that $\int |\phi(z)|\, dz$ is finite. Our concern is with the density matrix.

One can find a sequence of sharper bounds by writing

$$\int_0^s \phi(x(u))\, du = \frac{1}{N} \sum_{i=0}^{N} \int_0^s \phi(x(u_i))\, du_i \tag{15}$$

and applying the Jensen inequality separately on each u_i variable. Then

$$\langle x_1|I(s)|x_2\rangle \leqslant E^* \int_0^s \frac{du_i}{s}, \ldots, \int_0^s \frac{du_N}{s} \exp\left[\frac{s}{N}\sum_{i=1}^{N}\phi(x(u_i))\right] \quad (16)$$

Introduce the local "density of paths"

$$C(z\,|\,s) = \frac{1}{s}\int_0^s \delta(x(u)-z)\,du, \qquad \int C(z\,|\,s)\,dz = 1 \quad (17)$$

Then,

$$\langle x_1|I(s)|x_2\rangle = E^* \exp\left[s\int C(z\,|\,s)\phi(z)\,dz\right] \quad (18)$$

The UB is, for any N

$$\langle x_1|I(s)|x_2\rangle \leqslant E^*\left\{\int dz\, C(z\,|\,s)\exp\left[\frac{s}{N}\phi(z)\right]\right\}^N \quad (19)$$

This views the UB from the z integration viewpoint with $C(z\,|\,s)$ as the weight function. By the properties of means,[8] the bounds for large N are sharper. In fact, for large N

$$N\log\left\{\int dz\, C(z)\exp\left[\frac{s}{N}\phi(z)\right]\right\}$$
$$= N\log\left\{1 + \frac{s}{N}\int C(z\,|\,s)\phi(z)\,dz + \frac{s^2}{N^2}\frac{1}{2!}\int C(z)\phi^2(z)\,dz + \cdots\right\} \quad (20)$$

As $N\to\infty$ we obtain the exact result $s\int c(z\,|\,s)\phi(z)\,dz$. The cumulant expansion is obtained by putting $N=1$ after expanding the logarithm. However, one loses the UB character when one stops at a finite number of terms.

While we have a sequence of sharper bounds, no one of them gives the exact second-order term in an expansion on ϕ. The exact result is

$$\frac{s^2}{2}\int\int\langle x_1|C(z\,|\,s)C(z_1\,|\,s)|x_2\rangle\phi(z)\phi(z_1)\,dz\,dz_1 \quad (21)$$

where

$$\langle x_1|C(z\,|\,s)|x_2\rangle = E^* C(z\,|\,s) \quad (22)$$

The N center approximation gives

$$\frac{1}{2!}\left(\frac{s}{N}\right)^2\left\{N\int dz\,\langle x_1|C(z\,|\,s)|x_2\rangle\phi^2(z) + \frac{N(N-1)}{2}\right.$$
$$\left.\times\int\langle x_1|C(z\,|\,s)C(z_1\,|\,s)|x_2\rangle\phi(z)\phi(z_1)\,dz\,dz_1\right\} \quad (23)$$

which is exact only as $N\to\infty$.

Note that for $\phi(z) \geqslant 0$ one can get UB accurate to ϕ^2 by using the integral equation

$$\langle x_1|I(t)|x_2\rangle = \langle x_1|\rho_0(t)|x_2\rangle + \int_0^t ds \int \langle x_1|\rho_0(t-s)|x_3\rangle \phi(x_3)\langle x_3|I(s)|x_2\rangle\, dx_3 \tag{24}$$

Upon insertion of the UB for $I(s)$ on the right-hand side, the UB is accurate to ϕ^2. If ϕ is $\leqslant 0$ the UB gets converted to a lower bound.

We note a curious point for the case of one dimension. If $\phi(z) \geqslant 0$ with $\phi_0 \equiv \int \phi(z)\, dz$ one can view $\phi(z)/\phi_0$ as a weight for the z integration. This gives

$$\langle x_1|I(z)|x_2\rangle \leqslant E^* \int \phi(z)\, dz \exp\left[\phi_0 \int_0^s \delta(x(u) - z)\, du\right] \tag{25}$$

This is a superposition based on the known density matrix for a one-dimensional delta function. There is the obvious multipoint extension.

We consider next the sharper of Symanzik's UB. The integral can be scaled as

$$\langle x_1|I(s)|x_2\rangle = s^{-\epsilon/2} \int_{x_2/\sqrt{s}}^{x_1/\sqrt{s}} D_1 x \exp\left[s \int_0^1 \phi\left(\sqrt{s}\, x(u)\right)\right] \tag{26}$$

so that we can recover $I(s)$ from $I(1)$. For $s = 1$ the bound is

$$\int_{x_2}^{x_1} D_1 x \exp\left[\int_0^1 \phi(x(u))\, du\right] \leqslant \exp\left[\int_0^1 \ln\langle x_1|B_1(u)|x_2\rangle\, du\right] \tag{27}$$

where the key quantity is the function

$$\begin{aligned}\langle x_1|B_1(u)|x_2\rangle &= \int_{x_2}^{x_1} D_1 x \exp\left[\phi(x(u))\right] \\ &= \int dz \langle x_1|\rho_0(1-u)|z\rangle \exp\left[\phi(z)\right] \cdot \langle z|\rho_0(u)|x_2\rangle \end{aligned} \tag{28}$$

Here the role of the u integration is more pronounced.

$$\exp\left[\int_0^1 \ln B_1(u)\right] \leqslant \int_0^1 du\, B_1(u) \tag{29}$$

follows from the Jensen inequality by taking $B_1(u) = \exp[A(u)]$.

We can establish a multicenter generalization of this inequality. Let

$$\langle x_1|B_N(u_i, \ldots, u_N)|x_1\rangle = \int_{x_2}^{x_1} D_1 x \exp\left[\frac{1}{N} \sum_{i=1}^{N} \phi(x(u_i))\right] \tag{30}$$

Let

$$g(u, \ldots, u_N) = \sum_{i=1}^{N} \frac{\phi(x(u_i))}{N} - \ln\langle x_1|B_N(u_i \ldots u_N)|x_2\rangle \tag{31}$$

and use this in

$$\exp\left[\int_0^1 \cdots \int_0^1 du_i \ldots du_N \, g(u_i \ldots u_N)\right] \leqslant \int_0^1 \cdots \int_0^1 du_i \ldots du_N \exp[\, g(u_i \ldots u_N)] \tag{32}$$

Then

$$\int_{x_2}^{x_1} D_1 x \exp\left[\int_0^1 \phi(x(u))\, du\right] \leqslant \exp\left[\int_0^1 \cdots \int_0^1 du_i \ldots du_N \ln\langle x_1|B_N(u_i \ldots u_N)|x_2\rangle\right] \tag{33}$$

The UB can also be combined with trial actions, as shown by Symanzik and used by Bruch and Revercomb. Suppose the trial action is $\lambda\int_0^1\phi_T(x(u))\,du$, with $\phi_T(x)$ having a prescribed functional form. The simple UB is

$$\langle x_1|I(1)x_2\rangle \leqslant E^* \exp\left[\lambda\int_0^1 \phi_T(x(u)du)\right]\int dz\, C(z)\exp[\phi(z) - \lambda\phi_T(z)] \tag{34}$$

Of course, if $\lambda\phi_T(x) \equiv \phi(x)$, the UB is exact, so that if the trial is "near" to $\phi(x)$, the UB should be sharper than that based on the free action. Practically, we are more interested in whether there is improvement for $|\lambda| < 1$, for rather general $\phi_T(x)$. The answer is yes, provided the path integral is finite for the chosen $\phi_T(x)$. For, one may compute the change in the bound to first order in λ. Whatever its value, one may choose the sign of λ to decrease the bound. On the other hand, the expression is always positive, so that a lowest value is reached for some λ.

3. DOUBLE TIME BOUNDS

We now consider path integrals of the type

$$\langle x_1|I(\beta)|x_2\rangle = \int_{x_2}^{x_1} D_\beta x \exp\left\{\frac{1}{2}\int_0^\beta\int_0^\beta W[x(u) - x(u')]\, du\, du'\right\} \tag{35}$$

Scaling to the Debroglie length $\sqrt{\beta}$, we have

$$\langle x_1|I(\beta)|x_2\rangle = \beta^{-\epsilon/2}\int_{x_2/\sqrt{\beta}}^{x_1/\sqrt{\beta}} D_1 y \times \exp\left\{\frac{\beta^2}{2}\int_0^1\int_0^1 W\left[(y(u) - y(u'))\sqrt{\beta}\,\right] du\, du'\right\} \tag{36}$$

It suffices to evaluate $I(1)$and to make the replacements $W(z) \to \beta^2 W(z\sqrt{\beta}), x_1 \to x_1/\sqrt{\beta}$, and to supply the overall factor $\beta^{-\epsilon/2}$. Translation invariance implies, in addition

$$\langle x_1|I(1)|x_2\rangle = \langle x_1 - x_2|I(1)|0\rangle \tag{37}$$

Consider the UB that come about by treating both the u and u' variables according to Symanzik's idea. In addition, work with the free action. Then

$$\langle y|I(1)|0\rangle \leqslant E^* \int_0^1 du \int_0^1 du' \exp\left[\tfrac{1}{2} W(x(u) - x(u'))\right] \tag{38}$$

This involves free particle correlation functions:

$$\langle x_1|K_0(z)|x_2\rangle = E^* \int_0^1 \int_0^1 \delta(x(u) - x(u') - z)\, du\, du' \tag{39}$$

Then

$$\langle y|I(1)|0\rangle = \int dz \, \langle y|K_0(z)|0\rangle \exp\left[\frac{W(z)}{2}\right] \tag{40}$$

For $y = 0$ we have

$$\langle 0|K_0(z)|0\rangle = \frac{2^{\epsilon-1}}{(2\pi)^{\epsilon/2}} \int_0^\infty dx\, (1 + x^2)^{\epsilon - 3/2} \exp\left[-2z^2(1 + x^2)\right] \tag{41}$$

In particular, for $\epsilon = 3$ we have the simple expression

$$\langle 0|K_0(z)|0\rangle = (2\pi)^{-5/2} \exp(-2z^2)/|z| \tag{42}$$

The expression diverges as $z \to 0$ for $\epsilon > 1$. For $\epsilon = 2$ it goes as $\ln(1/|z|)$. For $\epsilon = 1$ it tends to the finite value $1/4$. For large $|z|$ it goes as $e^{-2z^2}/|z|$ for any dimension.

Another way to obtain this bound is to write [with $C(z) \equiv C(z \mid 1)$],

$$\langle y|I(1)|0\rangle = E^* \exp\left[\frac{1}{2} \int \int dz\, dz_1\, C(z) C(z + z_1) W(z_1)\right] \tag{43}$$

Note now that

$$\Phi(z) \equiv \int C(z_1) C(z + z_1)\, dz_1 \tag{44}$$

is normalized to unity:

$$\int \Phi(z)\, dz = 1 \tag{45}$$

$\Phi(z)$ can be considered as a weight for the z integration. This viewpoint is useful in calculations, and the results can be justified by going back to the u

integrations. We have

$$\langle y|I(1)|0\rangle \leqslant E^* \int dz \exp\left[\frac{W(z)}{2} \right] \Phi(z) \tag{46}$$

and

$$\int_0^y D_1 x \, \Phi(z) = \langle y|K_0(z)|0\rangle \tag{47}$$

The generalization to a multipoint bound is immediate. It is

$$\langle y|I(1)|0\rangle \leqslant E^* \left\{ \int \Phi(z) \exp\left[\frac{W(z)}{2N} \right] dz \right\}^N \tag{48}$$

This is less than the single point bound for any $N > 1$, and in the limit $N \to \infty$, we find the exact expression.

The stronger double time Symanzik bounds can easily be derived (as he already noted) by following the argument used in potential theory.

There is an elementary way of improving the UB so that it is accurate to order W^2. For any action A, we introduce a coupling constant g. We have the identity

$$\exp(A) - 1 = \int_0^1 dg \, A e^{gA} \tag{49}$$

The UB procedure is applied to the last term and one operates with E^*. For the double time UB this leads to

$$\begin{aligned} \langle y|I(1) - \rho_0(1)|0\rangle \leqslant \int\int dz \, dz_1 \left[\frac{W(z_1)}{W(z)} \right] \left\{ \exp\left[\frac{W(z)}{2} \right] - 1 \right\} \\ \times E^*\left[\Phi(z) \Phi(z_1) \right] \end{aligned} \tag{50}$$

4. SINGLE TIME BOUNDS

The bounds of the previous section are rather weak. They involve free-particle correlation functions. For example the bound is infinite if $W(x)$ is a one-dimensional delta function. Hence, we do not discuss improvement by the techniques described in the section on potential theory.

A more powerful result is obtained if one works on only one of the time variables. Thus

$$\langle y|I(1)|0\rangle \leqslant E^* \int_0^1 du \exp\left[\frac{1}{2} \int_0^1 W(x(u') - x(u)) \, du' \right] \tag{51}$$

Inserting, for given u, $1 = \int \delta(x(u) - z)\, dz$

$$\langle y|I(1)|0\rangle \leqslant E^* \int_0^1 du \int dz\, \delta(x(u) - z) \exp\left[\frac{1}{2} \int_0^1 W(x(u') - z)\, du' \right]$$

$$\leqslant E^* \int dz\, C(z) \exp\left[\frac{1}{2} \int W(z_1) C(z_1 + z)\, dz_1 \right] \tag{52}$$

Naturally, this can be obtained by using $C(z)$ as a weight for the z integration.

We need the potential type of density matrix

$$\langle y_1|R(s)|y_2\rangle = E^* \exp\left[\frac{1}{2} \int_0^s W(x(u))\, du \right] \tag{53}$$

Here the potential is centered at the origin. Then

$$\text{(A)} \quad \langle y|I(1)|0\rangle \leqslant dz \int_0^1 \langle y + z|R(1 - s)|0\rangle\langle 0|R(s)|z\rangle\, ds$$

$$\leqslant \int \frac{dk}{(2\pi)^\epsilon} \exp(-iky) \tilde{R}(-k\,|\,1 - s) \tilde{R}(k\,|\,s) \tag{54}$$

in terms of the spatial Fourier transform.

In particular, for $y = 0$, we have the simple result

$$\text{(A}'\text{)} \qquad \langle 0|I(1)|0\rangle = \langle 0|R(1)|0\rangle \tag{55}$$

(A) and (A′) are the most useful results of the UB analysis. The generalization to a multipoint bound is immediate. It is

$$\langle y|(1)|0\rangle \leqslant E^* \left\{ \int dz\, C(z) \exp\left[\int C(z + z_1) W(z_1)\, dz_1 / 2N \right] \right\} \tag{56}$$

We now need an N-center single-particle density matrix

$$\langle y_1|R_N(z_i, \ldots, z_N \,\|\, s)|y_2\rangle = E^* \exp\left\{ \sum_{i=1}^N \int_0^s W(x(u) - z_i)\, du / 2N \right\} \tag{57}$$

The bound is

$$\begin{aligned} \langle y|I(1)|0\rangle \leqslant N! \int_0^1 du_1 \int_0^{u_1} du_2 \ldots \int dz_i \ldots \int dz_N & \\ \times \langle y|R_N(z_i \ldots z_N \,\|\, 1 - u_1)|z_i\rangle & \\ \times \langle z_i|R_N(z_i \ldots z_N \,\|\, u_1 - u_2)|s\rangle \ldots & \\ \times \langle z_N|R_n(z_i \ldots z_N \,\|\, u_N)|0\rangle & \end{aligned} \tag{58}$$

Note that the z_i variables enter both into the end points of the matrix elements and as the values of the centers of the potential. So this is not simple matrix multiplication.

We refer to the preceding as symmetrical bounds. There are other, asymmetrical, ones. A second type is based on writing the action as

$$\frac{1}{2}\int_0^1 du \int_0^1 du'\, W(x(u) - x(u')) = \int_0^1 du \int_0^u du'\, W(x(u') - x(u)) \tag{59}$$

Again, we insert a delta function in the path integral

$$\langle y|I(1)|0\rangle \leqslant E^* \int_0^1 du \int dz\, \delta(x(u) - z) \exp\left[\int_0^u du'\, W(x(u') - z)\right] \tag{60}$$

This involves the same type potential as in the symmetric case, but with double the strength. To avoid confusion we use the separate notation

$$\langle x_1|\, Q_1(z\,|\,u)|x_2\rangle = E^* \exp\left[\int_0^u du'\, W(x(u') - z)\right] \tag{61}$$

In decomposing the expression, note that the stretch from 1 to u involves the free-particle density matrix.

$$\text{(B)} \qquad \langle x_1|I(1)|0\rangle \leqslant \int dz \int_0^1 du_1 \langle x_1|\rho_0(1 - u)|z\rangle\langle z|\, Q_1(z\,|\,u)|0\rangle \tag{62}$$

The generalization to $N = 2$ is

$$\begin{aligned}\langle x_1|I(1)|0\rangle \leqslant 2\int dz_2 \int_0^1 du_1 \int du_2 \langle y_1|\rho_0(1 - u_1)|z_1\rangle\langle z_1|R_1(z_1|u_1 - u_2)|z_2\rangle \\ \times \langle z_2|\, Q_2(z_1, z_2\,|\,u_2)|0\rangle\end{aligned} \tag{62'}$$

Here

$$\langle z_2|\, Q_2(z_1, z_2\,|\,u)|0\rangle = E^* \exp\left\{\frac{1}{2}\int_0^u [\, W(x(u') - z_1) + W(x(u') - z_2)]\, du'\right\} \tag{63}$$

We now examine the relation between the two types of bound. The (B) form comes from

$$\begin{aligned}\langle 0|I(1)|0\rangle \leqslant E^* \sum_{n=0}^{\infty} \int_0^u du_1 \int_0^{u_1} du_2 \ldots \\ W[x(u_1) - x(u)] \ldots W[x(u_n) - x(u)]\end{aligned} \tag{64}$$

The $1/n!$ from the exponential is canceled by the $n!$ arrangements. This is

$$\langle 0|I(1)|0\rangle \leqslant E^* \sum_{n=0}^{\infty} \frac{1}{(n+1)!}\left[\int_0^1 W(z(u') - x(u))\, du'\right]^n \tag{65}$$

Since

$$\frac{1}{2n}\,\frac{1}{2!} \leqslant \frac{1}{(n+1)!}$$

we have the result that for $W > 0$, the (A) bound is sharper. On the other hand for $W < 0$, there are alternating signs and we have no conclusion.

5. USE OF HIERARCHY

By an argument like that used in potential theory, one sees that the UB do not give the W^2 terms of perturbation theory correctly. To get bounds which do agree, we need bounds for correlation functions.

There is a hierarchy linking $\langle x_1|I(t)|x_2\rangle$ to correlation functions. It is derived by the standard integration by parts technique used in path integral theory.[4] Here we write

$$\exp[A(t)] - \exp[A(0)] = \int_0^t ds \frac{\partial}{\partial s} \exp[A(s)]$$
$$= \int_0^s ds \frac{\partial A(s)}{\partial s} \exp[A(s)] \tag{66}$$

We apply this to

$$A(s) = \int_0^s ds_1 \int_0^{s_1} W(x(s_1) - x(s_2))\, ds_2 \tag{67}$$

This gives the first hierarchy equation

$$\langle x_1|I(t) - \rho_0(t)|x_2\rangle = s\int_0^t ds \int \langle x_1|\rho_0(t-s)|z\rangle dz\, W(y-z)\langle z|I_1(y\mid s)|x_2\rangle \tag{68}$$

where

$$\langle z|I_1(y\mid s)|x_2\rangle \equiv \int_{x_2}^{z} D_s x\, C(y\mid s)\exp[A(s)] \tag{69}$$

If $W \geqslant 0$, an upper bound for $I_1(y\mid s)$ yields an upper bound for $I(s)$. To derive such a bound, we first use $C(z\mid s)$ as a weight for the z integration. This gives the symmetrical UB

$$\langle x_1|I(y\mid s)|x_2\rangle \leqslant E^* C(y\mid s)\int dz\, C(z\mid s)\exp\left[\frac{s^2}{2}\int dz_1\, C(z_2)W(z_1 - z)\right] \tag{70}$$

We now need a density matrix

$$\langle x_1|P_t(z\mid s)|x_2\rangle \equiv E^* \exp\left[\frac{t}{2}\int_0^s W(x(u) - z)\, du\right] \tag{71}$$

evaluated at $t = s$. Note that $P_1(0\mid s) = R(s)$, $P_2(0\mid s) = Q_1(0\mid s)$.

One finds the bound

$$\langle x_1|I_1(y\,|\,s)|x_2\rangle \leqslant \int_0^s \frac{du}{s}\int_0^u \frac{du}{s}\,dz\,\big[\langle x_1|P_s(z\,|\,s-u)|y\rangle\langle y|P_s(z\,|\,u-u')|z\rangle \times \langle z|P_s(z\,|\,u')|x_2\rangle + \langle x_1|P_s(z\,|\,s-u)|z\rangle \times \langle z|P_s(z\,|\,u-u')|y\rangle\langle y|P_s(z\,|\,u')|x_2\rangle\big] \tag{72}$$

The hierarchy equations are usually treated by Laplace transforms on the time variables. The dependence of the strength of the potential on the s variables then leads to severe complications.

The second, asymmetrical technique may also be used to evaluate the correlation functions needed for the first hierarchy equation:

$$\langle x_1|I_1(y\,|\,s)|x_2\rangle \leqslant E^*\int_0^s \frac{du}{s}\int_0^s \frac{du_2}{s}\,\delta(x(u_2)-y)\delta(x(u)-z) \times \exp\left[s\int_0^u W(x(u_1)-z)\,du_1\right] \tag{73}$$

The action now has twice the strength of the previous action:

$$\langle x_1|\Phi(y\,|\,s)|x_2\rangle \leqslant 2\int_0^s \frac{du}{s}\int_0^u \frac{du_2}{s}\int dz\big[\langle x_1|\rho_0(s-u)|z\rangle \times \langle z|P_{2s}(u-u_2)|y\rangle \times\langle y|P_{2s}(z\,|\,u_2)|x_2\rangle + \langle x_1|\rho_0(s-u)|y\rangle \times\langle y|P_{2s}(z\,|\,u-u_2)|z\rangle\langle z|P_{2s}(z\,|\,u_2)|x_2\rangle\big] \tag{74}$$

Note that one of the factors is the free-particle density matrix.

Naturally, this can easily be generalized to the multipoint bounds. But the practical value is doubtful.

Finally we note that for the one-dimensional case, if $W(z)$ is $\geqslant 0$ and $W_0 = \int W(z)\,dz$ is finite, we can use $W(z)/W_0$ as a weight for the z integration. Then we have an upper bound based on a superposition of two time delta function actions.

To obtain bounds accurate to W^2, we can also use the coupling constant integration. Then

$$\langle y|I(1)-\rho_0(1)|0\rangle \leqslant \int_0^1 dg\int\int dz\,dz_1\,W(z_1) \times E^*\left\{\Phi(z_1)C(z)\exp\left[g\int W(z_2-z)C(z_2)\,dz_2\right]\right\} \tag{75}$$

This also involves three Pg factors.

6. TEST OF BOUNDS ON SOLUBLE CASE

To examine the nature of the upper bounds, we study the soluble action

$$A(\beta) = \frac{-\Omega^2}{4}\int_0^\beta\int_0^\beta [x(u) - x(u')]^2\,du\,du' \tag{76}$$

$$\langle y_1|I(\beta\,|\,\Omega)|y_2\rangle = E^* \exp[A(\beta)] \tag{77}$$

From the translation invariance of $A(\beta)$, the value of I depends only on the difference $y_1 - y_2$. For the one-dimensional case, scaling to the thermal deBroglie length yields

$$\langle y|I(1\,|\,\Omega)|0\rangle = \beta^{-1/2}\langle y/\sqrt{\beta}\,|I(1\,|\,\Omega\beta^{3/2})|0\rangle \tag{78}$$

so that it suffices to evaluate $\langle y|I(1\,|\,\Omega)|0\rangle$.

The action $A(1)$ can be written as

$$A(1) = \frac{-\Omega^2}{2}\int_0^1 x^2\,du + \frac{\Omega^2}{2}\left(\int_0^1 x\,du\right)^2 \tag{79}$$

Using a parametric representation for the exponential of the last term, and the theory of the forced harmonic oscillator, one finds the exact result[9]

$$\langle y|I(1\,|\,\Omega)|0\rangle = \frac{1}{\sqrt{2\pi}}\left(\frac{\Omega}{2}\Big/\sinh\frac{\Omega}{2}\right)\exp\left[\frac{-\Omega}{4}\left(\coth\frac{\Omega}{2}\right)y^2\right] \tag{80}$$

Consider first the case $y = 0$. The single point symmetric Symanzik UB is (with $\omega = \Omega/\sqrt{2}$)

$$\langle 0|I(1\,|\,\Omega)|0\rangle \leqslant \frac{1}{\sqrt{2\pi}}\left(\frac{\omega}{\sinh\omega}\right)^{1/2} \tag{81}$$

In the limit $\omega \to \infty$ there is a discrepancy for both the dominant exponential and for the prefactor.

It is also possible to calculate the two point UB. We find

$$\langle 0|I(1\,|\,\Omega)|0\rangle \leqslant 4\int_0^1 du\,(1-u)\,dz\,\langle z|\rho(1-u\,|\,\omega)|-z\rangle$$

$$\times\langle z|\rho(u\,|\,\omega)|-z\rangle \exp\left(\frac{-\omega^2 z^2}{2}\right) \tag{82}$$

$\rho(u\,|\,\omega)$ is the density matrix for an oscillator of angular frequency ω.

Carrying out the z integration, one finds

$$\langle 0|I(1\,|\,\Omega)|0\rangle \leqslant 2\Big(\frac{\omega}{\pi}\Big)^{1/2}\int_0^1 du\,(1-u)\Big[\,\frac{\omega}{2}\sin\omega u\sinh\omega(1-u)+\sinh\omega + \sinh\omega u+\sinh\omega(1-u)\Big]^{-1/2} \tag{83}$$

In the limit of large ω, the contribution from the ground state dominates, and

$$\langle 0|I(1\,|\,\Omega)|0\rangle \leqslant \Big(\frac{2\omega}{\pi}\,\frac{1}{1+\omega/4}\Big)^{1/2}\exp(-\omega/2) \tag{84}$$

The improvement is only in the prefactor, and not in the dominant exponential. The $N\to\infty$ limit (for fixed ω) must be taken to get the exponential term correctly. For given, large N, the accuracy decreases for sufficiently large ω.

The asymmetrical one-point UB is less sharp. We have

$$\langle 0|I(1\,|\,\Omega)0\rangle \leqslant \Big(\frac{\Omega}{2\pi}\Big)^{1/2}\int_0^1 du\,\big\{\sinh\Omega u\big[1+(1-u)\Omega\cosh\Omega u\big]\big\}^{-1/2} \tag{85}$$

For large Ω this has an inverse power behavior. This is true for the weaker, double time bounds.

For $y\neq 0$, the symmetrical one-point bound is

$$\langle y|I(1\,|\,\Omega)|0\rangle \leqslant \Big(\frac{\omega}{2\pi}\sinh\omega\Big)^{1/2}\int_0^1 du\exp\Big[\frac{-\omega y^2}{2}\,\frac{\cosh\omega u}{\cosh\omega(1-u)+\cosh\omega u}\Big] \tag{86}$$

When $\omega\to\infty$ the exponential fall off, $\exp(-\omega y^2/4)$, is slower than the exact result, $\exp(-\omega\sqrt{2}\,y^2/4)$.

For this soluble action, the lower bounds are more accurate.[9] Since

$$A(1) \geqslant \frac{-\Omega^2}{2}\int_0^1 x^2\,du \tag{87}$$

$$\langle 0|I(1\,|\,\Omega)|0 \leqslant (\Omega/2\pi\sinh\Omega)^{1/2} \tag{88}$$

This has the correct exponential term, but an incorrect prefactor. When the prefactor is put into the exponential, this translates to an incorrect coefficient for the $\log\Omega$ term. The use of the Jensen inequality with the oscillator action leads to a better lower bound. There is an extra positive term in the exponential. This term is

$$\frac{\omega^2}{2}\int_0^1 D_1x\Big(\int_0^1 x(u_1)\,du_1\Big)^2\exp\Big[\frac{-\omega^2}{2}\int_0^1 y^2\,du\Big]\Big/\langle 0|\rho(1\,|\,\omega)|0\rangle \tag{89}$$

For large ω this leads to an ω^0 correction and thus does not affect the logarithmic term.

7. THE ONE-DIMENSIONAL DELTA FUNCTION

In the present section we examine the two time action involving a one-dimensional delta function, viz.,

$$\langle y|J(1)|0\rangle = E^* \exp\left[\frac{\gamma}{2}\int_0^1\int_0^1 \delta(x(u)-x(u'))\,du\,du'\right] \tag{90}$$

As noted earlier, the double time UB is infinite. The symmetric single time UB is for $y=0$

$$\langle 0|J(1)|0\rangle \leqslant E^* \exp\left[\frac{\gamma}{2}\int_0^1 \delta(x(u))\,du\right] \equiv \langle 0|R(1)|0\rangle \tag{91}$$

Explicitly

$$\langle 0|J(1)|0\rangle \leqslant \frac{1}{2\sqrt{2\pi}} + \frac{\gamma}{4}\exp(\gamma^2/8)\operatorname{erfc}\left(\frac{-\gamma}{2\sqrt{2}}\right)$$

$$\operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}}\int_z^\infty dt\,\exp(\gamma^2) \tag{92}$$

As $\gamma \to \infty$

$$\langle 0|J(1)|0\rangle \leqslant \frac{1}{\sqrt{2\pi}} + \frac{\gamma}{2}\exp\left(\frac{\gamma^2}{8}\right) \tag{93}$$

The first term is the free-particle contribution. The second term is the contribution from the bound state for a particle in an attractive delta function potential. The energy is $E_0 = -\frac{1}{2}(\gamma/2)^2$ and the wave function is $\chi_0(x) = \sqrt{\gamma/2}\exp(-|x|\gamma/2)$. The distortion of the continuum states is a correction to the dominant term. One knows, from lower bound estimates,[9] and from systematic asymptotic theory, that for $\gamma \to \infty$, the exponent is $\gamma^2/24$. So there is the same dependence on γ, but the coefficient of the upper bound is larger by a factor of 3. For $\gamma \to 0$, $J(1)$ has an expansion in powers of γ. In accord with the general analysis the first power of γ is exact and the second power of γ is too large.

The asymmetrical upper bound is

$$\langle 0|J(1)|0\rangle \leqslant \int_0^1 du \int dz\,\langle 0|\rho_0(1-u)|z\rangle\langle z|\,Q(u)|0\rangle \tag{94}$$

$$\langle z|\,Q(u)|0\rangle \equiv E^* \exp\left[\gamma\int_0^1 \delta(x(u))\,du\right] \tag{95}$$

One can use the integral equation obeyed by $Q(u)$ to reach the simpler form

$$\langle 0|J(1)|0\rangle \leqslant \frac{1}{(2\pi)^{1/2}} + \frac{\gamma}{(2\pi u)^{1/2}} \int_0^1 du\,(1-u)^{1/2} \langle 0|\,Q(u)|0\rangle \tag{96}$$

In the limit of large γ, $(1-u)^{1/2}$ can be replaced by 1. The behavior is governed by the bound state with twice the strength, viz., $\exp(\gamma^2/2)$. Again this is a weaker bound, in accord with the general analysis.

We now examine the spatial behavior of the symmetric UB

$$\langle y|J_T(t)|0\rangle = \int dz \int_0^t ds\, \langle x+z|R(t-s)|0\rangle\langle 0|R(s)|z\rangle \tag{97}$$

We take the Laplace transform

$$\langle x_1|\bar{R}(p)|x_2\rangle = \int_0^\infty e^{-pu}\langle x_1|R(u)|x_2\rangle\, du \tag{98}$$

and use the convolution theorem. All transforms have the same p value so that we frequently suppress this argument. Then

$$\langle y|\bar{J}_T|0\rangle = \int dz \langle y+z|\bar{R}|0\rangle\langle 0|\bar{R}|z\rangle \tag{99}$$

For the one-dimensional delta function,

$$\langle 0|\bar{R}|z\rangle = \langle 0|\bar{\rho}_0|z\rangle \frac{\sqrt{p}}{\sqrt{p} - \gamma/2\sqrt{2}} \tag{100}$$

$$\langle 0|\bar{\rho}_0|z\rangle = \exp\left[-|z|(2p)^{1/2}\right]/(2p)^{1/2} \tag{100$'$}$$

The Markov property, that for any s,

$$\int dx_3 \langle x_1|\rho_0(t-s)|x_3\rangle\langle x_3|\rho_0(s)|x_2\rangle = \langle x_1|\rho_0(t)|x_2\rangle \tag{101}$$

become in transform space

$$\int dz\, \langle x_1 + z|\bar{\rho}_0(p)|0\rangle\langle 0|\bar{\rho}_0(p)|z\rangle = \frac{-\partial}{\partial p} \langle 0|\bar{\rho}_0(p)|x_1\rangle \tag{102}$$

Hence

$$\langle y|\bar{I}_T(\rho)|0\rangle = \frac{-p}{\left(\sqrt{p} - \gamma/2\sqrt{2}\right)^2} \frac{\partial}{\partial p} \langle 0|\bar{\rho}_0(p)|y\rangle \tag{103}$$

Using the table of Laplace transform inverses,[10] and evaluating at $t = 1$,

$$\begin{aligned}\langle y|J_T(1)|0\rangle = \exp\left(\frac{-\gamma^2}{2}\right) \frac{1}{(2\pi)^{1/2}} \left(1 + \frac{\gamma}{2}|y|\right) \\ + \frac{\gamma}{4}\left(1 + \frac{\gamma}{2}|y| - y^2\right) \exp\left(\frac{-y^2}{2}\right) H\left(\frac{|y| - \gamma/2}{\sqrt{2}}\right)\end{aligned} \tag{104}$$

where

$$H(z) = \exp(z^2/2)\mathrm{erfc}(z) \tag{105}$$

There is only a small change from free-particle behavior when $x \gg 1$. In particular the long tail from weakly bound state for $\lambda < 1$ is washed out. We will simply set down the formulas for the two-point UB. Here the two-center density matrix is

$$\langle x_1|R_2(z_1,z_2\,|\,t)|x_2\rangle = E^* \exp\left\{ \frac{\gamma}{4}\int_0^t \left[\delta(x(u)-z_1) + \delta(x(u)-z_2)\right] du \right\} \tag{106}$$

The Laplace transforms needed are $[q = (2p)^{1/2}]$

$$\begin{aligned} \langle z_1|\bar{R}_2(z_1,z_2\,|\,p)|z_2\rangle &= \exp(-q|z_2 - z_1|)/q\Delta \\ \langle z_2|\bar{R}_2(z_1,z_2\,|\,p)|0\rangle &= \frac{1}{q}\left(1-\frac{\gamma}{4q}\right)\exp[-q\,|\,z_2] \end{aligned} \tag{107}$$

Here

$$\begin{aligned} \Delta = \left(1-\frac{\gamma}{4q}\right)^2 - \left(\frac{\gamma}{4}\right)^2 \frac{1}{q^2}\exp[-2q\,|\,z_2 z_1] \\ + \left(\frac{\gamma}{4}\right)^2 \frac{1}{q^2}\exp[-q|z_1| - q|z_1+z_2|] \end{aligned} \tag{108}$$

This is to be used in

$$\begin{aligned} \langle 0|\bar{J}_T(p)|0\rangle = 2!\int\int dz_1\,dz_2 \langle 0|\bar{R}_2(z_1,z_2)|z_1\rangle \\ \times \langle z_1|\bar{R}_2(z_1,z_2)|z_2\rangle\langle z_2|\bar{R}_2(z_1,z_2)|0\rangle \end{aligned} \tag{109}$$

The evaluation of the inverse transform is difficult.

8. SHELL CORRELATION FUNCTIONS

We first restate the content of the UB (A) and (A′). In ordinary units

$$\langle y|I(\beta)|0\rangle = E^* \exp\left[\frac{1}{2}\int_0^\beta\int_0^\beta W(x(u) - x(u'))\,du\,du'\right] \tag{110}$$

We introduced

$$\langle x|P_t(z\,|\,s)|x\rangle = E^* \exp\left[\frac{t}{2}\int_0^s W(x(u) - z)\,du\right] \tag{71}$$

Then (A) and (A′) are

$$\langle y|I(\beta)|0\rangle \leqslant \frac{1}{\beta}\int_0^\beta ds\int dz\,\langle y+z|P_\beta(0\,|\,\beta - s)|0\rangle\langle 0|P_\beta(s)|z\rangle \tag{111}$$

$$\langle 0|I(\beta)|0\rangle \leqslant \langle 0|P[(0\,|\,\beta)|0]\rangle \tag{112}$$

We now study these bounds for correlation functions $W(x) = V_0 f(x)$, $\int f(x)\, d^{\epsilon}x = 1$, $f(x) \geqslant 0$ where the correlation length in $f(x)$ is unity. We have a short-range attractive potential with a β-dependent strength. There is a significant dependence on dimensionality when $V_0 \beta \ll 1$. There are bound states in one and two dimensions.[11,12] The behavior can be studied in detail for shell potentials and for potential holes.

It is expedient to introduce

$$\langle x_1 | L_\lambda(s) | x_2 \rangle = E^* \exp\left[\lambda \int_0^s f(x(u))\, du \right] \tag{113}$$

Here, when $\lambda = V_0 \beta / 2$, $L_\lambda(s) = P_\beta(0 \mid s)$. Then

$$\beta \langle y | I(\beta) | 0 \rangle \leqslant \int_0^\beta ds \int dz \, \langle y + z | L_\lambda(\beta - s) | 0 \rangle \langle 0 | L_\lambda(s) | z \rangle \tag{114}$$

The problems will be analyzed by taking the Laplace transform of $L_\lambda(s)$. After taking the inverse, we set $\lambda = V_0 \beta / 2$.

The integral equation for the transform is

$$\langle x_1 | \bar{L}_\lambda | x_2 \rangle = \langle x_1 | \bar{\rho}_0 | x_2 \rangle + \lambda \int \langle x_1 | \bar{\rho}_0 | x_3 \rangle f(x_3) \langle x_3 | \bar{L}_\lambda | x_2 \rangle \, dx_3 \tag{115}$$

In one dimension the transform exists even when $x_1 = x_2 = 0$. We consider the one-dimensional "shell" potential

$$f(x) = \tfrac{1}{2} \left[\delta(x - 1) + \delta(x + 1) \right] \tag{116}$$

We find $[q = (2p)^{1/2}]$

$$\langle x | \bar{L}_\lambda | 0 \rangle = \frac{\exp(-q|x|)}{q} + \lambda \bar{F} \frac{\left[\exp(-q|x+1|) + \exp(-q|x-1|) \right]}{2q} \tag{117}$$

where

$$\bar{F} = \exp(-q) \Big/ \left\{ q - \frac{\lambda}{2} \left[1 + \exp(-2q) \right] \right\} \tag{118}$$

If $\lambda \ll 1$ there is a bound state at $q = \lambda$, $p = \lambda^2/2$. It contributes to $\lambda \exp(-\lambda + \lambda^2 s/2)$ to $\langle 0 | L_\lambda(s) | 0 \rangle$. However, this is contained in the perturbation series in powers of λ. On the other hand, $\lambda \gg 1$ the bound state is at $q = \lambda/2$, $p = \frac{1}{2}(\lambda/2)^2$, and

$$\langle 0 | L(s) | 0 \rangle \to \frac{1}{(2\pi s)^{1/2}} + \lambda e^{-\lambda} \exp\left(\frac{\lambda^2 s}{8} \right) + \cdots \tag{119}$$

One can verify that the dominant term comes from the bound state which is determined by the condition

$$q(1 + \tanh q) = \lambda \tag{120}$$

To study the spatial behavior of the UB one must examine

$$\overline{M}(x) = \frac{1}{2\pi}\int \exp(-ikx)|\tilde{\bar{L}}(k)|^2\,dk \tag{121}$$

Here

$$\tilde{\bar{L}}(k) = \frac{1}{p + k^2/2}\left[1 + \lambda\cos(k)\cdot\overline{F}\right] \tag{122}$$

The approach to the one-dimensional delta function is to put $\cos(k)$ and the exponentials in $\overline{F}$ equal to unity. The most important question is the contribution of the bound state to the spatial behavior. For large $|x|$ we may put $\cos(k)$ equal to unity. Let $F(s)$ and $F_2(s)$ be the Laplace inverses of $\overline{F}(p)$ and $[\overline{F}(p)]^2$. Then we may use the convolution theorem.

$$M_\lambda(x\,|\,t) = (2\pi t)^{-1/2}\exp(-x^2/2t) + \frac{1}{(2\pi)^{1/2}}$$
$$\times\int_0^t (t-s)^{1/2}\exp\left(\frac{-x^2}{2|t-s|}\right)ds\left[2\lambda F(s) + \lambda^2 F_2(s)\right] \tag{123}$$

The way in which the contribution of the bound state is washed out by the free-particle factor is a general feature.

Consider the two-dimensional shell potential

$$f(r) = \frac{1}{2\pi}\delta(r-1) \tag{124}$$

We use the partial wave decomposition

$$\langle \mathbf{x}_1|\overline{L}|\mathbf{x}_2\rangle = \frac{1}{(2\pi)^2}\sum_{m=-\infty}^{+\infty}\langle r_1|\overline{L}_m|r_2\rangle\exp\left[im(\phi_1-\phi_2)\right] \tag{125}$$

and the same decomposition for $\bar{\rho}_0$. Then

$$\langle r_1|\bar{\rho}_{0,m}|r_2\rangle = 4\pi I_m(qr_1)K_m(qr_2) \qquad \text{if} \quad r_1 < r_2 \tag{126}$$

in terms of modified Bessel functions. The solution is

$$\langle r_1|\overline{L}_m|r_2\rangle = \langle r_1|\bar{\rho}_{0,m}|r_2\rangle + \frac{\lambda}{2\pi}\frac{\langle r_1|\bar{\rho}_{0,m}|1\rangle\langle 1|\rho_{0,m}|r\rangle}{\left[1 - 2\lambda I_m(q)K_m(q)\right]} \tag{127}$$

The bound states are given by the solutions of

$$1 = 2\lambda I_m(q)K_m(q) \tag{128}$$

There is at most one bound state for each m. It exists, for $m = 0$, even when $\lambda \to 0$. Then

$$p \to p^* \to 2\exp(-1/\lambda - 2\gamma^*) \tag{129}$$

where $\gamma^* = 0.5772$ is the Euler constant. This nonanalytic contribution is not recoverable from the perturbation series in λ.

For $r_1 = r_2 < 1$ and $r_1 \to 0$, the only $m = 0$ term contributes:

$$\langle 0|L_\lambda(t)|0\rangle \to \frac{1}{2\pi t} + 2\lambda^3 K_0^2(\lambda)\exp\left(\frac{\lambda^2}{2}\right) \tag{130}$$

with

$$K_0(\lambda) \to (\pi/2\lambda)^{1/2}\exp(-\lambda) \tag{131}$$

When r_1 or $r_2 \neq 0$, the $m \neq 0$ states contribute. For large λ the bound states differ from the $m = 0$ state by an amount independent of λ. Thus they contribute to the prefactor of the dominant term. To determine the spatial behavior of the UB for the original two time Wiener integral, we need to study the space and time convolutions, as sketched for the one-dimensional shell case. We have not studied this in detail.

Another case that can be done is a correlation function that is constant over a small range, i.e., a potential well of depth V_0. There is an important difference in the $\lambda \gg 1$ limit. For deep potential wells the low-lying states have eigenvalues given by the depth of the well plus the eigenvalues of a particle in an infinitely high box. For example in the one-dimensional case

$$\langle 0|L_\lambda(t)|0\rangle \to 2\sum_{n=0}^{\infty} \sin^2\left(\frac{n\pi}{2}\right)\exp\left(\frac{-n^2\pi^2 t}{2}\right)\exp(\lambda t) \tag{132}$$

Th sum is over all states whose eigenfunctions are nonvanishing at the origin. The leading term has an exponential dependence on λ rather than on λ^2, as was the case for the more singular shell potentials and one-dimensional delta function. Clearly this feature is independent of the dimension. The limiting dependence on λ is also characteristic of smooth correlation functions.

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