Journal of Statistical Physics, Vol. 33, No. 1, 1983

Partition Function of a Particle Subject to Gaussian Noise

Eugene P. Gross[1]

Received April 5, 1983

We study the averaged partition function for a quantum particle subjected to Gaussian noise using the path integral representation. The noise is characterized by a covariance function with a strength and a range. It falls off rapidly with distance but the analytic form at short distances and the dimensionality are important. The remaining parameter is the thermal length of the particle. For a finite range we study the behavior of the partition function over the entire domain of strengths and thermal lengths. The techniques used are successively more accurate upper and lower bounds that include contributions from configurations involving traps. Particular attention is paid to a self-consistent field analysis lower bound and to a nonlocal quadratic action bound. We also study the white noise limit, i.e., vanishing range with finite values of the other parameters. In one dimension the white noise limit leads to convergent results. In three or higher dimensions the divergent terms can be isolated and computed. In two dimensions the degree of divergences changes at a finite value of the product of the strength and thermal length squared.

KEY WORDS: Partition function; path integral; Gaussian noise.

1. INTRODUCTION

The density matrix describes some important properties of a particle subject to a potential $V(x)$. In the path integral representation, with units $\hbar = m = 1$

$$\langle x_1|\rho(\beta)|x_2\rangle = \int_{x_2}^{x_1} D_\beta x \exp\left[-\int_0^\beta V(x(u))\,du\right] \tag{1}$$

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

0022-4715/83/1000-0107$03.00/0

Here

$$D_\beta x \equiv \mathscr{D}_\beta x \exp\left[-(1/2)\int_0^\beta \left(\frac{dx}{du} \right)^2 du \right] \tag{2}$$

is the Wiener measure.

β need not be the physical inverse temperature of a heat bath. It may be a parameter. The density of states and momentum spectral density can be obtained by taking the inverse Laplace transform of the density matrix.

The density matrix for the potential problem obeys the Bloch differential equation. This is the simplest approach to finding $\rho(\beta)$ when the potential is a δ function, a hard core, or is spatially localized. It is also the natural way to bring in the theory of differential equations, eigenfunction analysis, etc. On the other hand, the path integral (P.I.) approach leads to new analysis of the semiclassical limit. There are also approximation methods specific to the P.I., such as the mean path analysis of Feynman and Hibbs,[1] the lower bound Feynman variational principle,[2] and the Symanzik upper-bound technique.[3]

We will consider the case where $V(x)$ is a random potential governed by a Gaussian probability distribution. The covariance is

$$\overline{V(x)V(y)} = W(x-y) = W_0 f\left(\frac{x-y}{L} \right) \tag{3}$$

The bar indicates an average with the probability distribution. We will consider monotonic functions $f(x)$ so that the covariance involves a length L and a strength W_0. The analytic form of $f(x)$, e.g., $\exp(-|x|)$, $\exp(-x^2)$, $\theta(1-|x|)$, $\delta(x)$ is also important.

Using the characteristic functional for a Gaussian process, the averaged density matrix is

$$\langle x_1|\bar{\rho}|x_2\rangle = \int_{x_2}^{x_1} D_\beta x \exp\left[\frac{1}{2} \int_0^\beta \int_0^\beta W(x(u) - x(u'))\, du\, du' \right] \tag{4}$$

We refer to the argument of the exponential as the "action." Since the action is invariant under the rigid translation $x(u) \to x(u) + x_2$, $\bar{\rho}$ depends only on $x_1 - x_2$. The diagonal element $\langle x_1|\bar{\rho}|x_1\rangle$ is independent of x_1. Thus the trace, i.e., the partition function, is proportional to the volume occupied by the system. In the following we omit this factor and also drop the bar that refers to the average.

The Gaussian random process can be considered as a limiting case of Poisson randomness. Let $V(x) = \sum_{i=1}^N v(\mathbf{x} - \mathbf{R}_i)$, where $\mathbf{R}_i$ is a site vector for an impurity, as in semiconductor physics. The atomic potential $v(x)$ has a strength and a range. If the site positions are uncorrelated the averaged density matrix can be written as an explicit P.I. using the characteristic functional of a Poisson process.[4-6] It involves the density of the impurities as well as the strength and range of the potential. This three-parameter problem reduces to a two-parameter Gaussian process at high densities. When $v(x)$ is a screened Coulomb potential, L is screening length and W_0 is proportional to the density of impurities as well as to L. The function $f(x)$ takes the form $\exp[-|x|]$.

Still available is the choice of a unit of length, and we will take $L = 1$ and write

$$W(x) = g^2 f(x). \tag{5}$$

The partition function (per unit volume) may be scaled to the de Broglie length. It is

$$\langle 0|\rho(\beta)|0\rangle = \beta^{-d/2}\int_0^0 D_1 x \exp\left(\frac{g^2\beta^2}{2}\int_0^1\int_0^1 f\left\{\sqrt{\beta}\left[x(u) - x(u')\right]\right\} du\, du'\right) \tag{6}$$

This shows that if $f(x)$ approaches a one-dimensional δ function, the partition function is the free particle $(2\pi\beta)^{-1/2}$ multiplied by a function of $g^2\beta^{3/2}$. In general, whenever the characteristic functional of the random process is known, we can directly see the dependence of the averaged density matrix on the parameters describing the process. This is a special case of the more general elimination of degrees of freedom coupled to a particle that was first highlighted by Feynman in his approach to quantum electrodynamics. The price that must be paid is the occurrence of a "multitime" action. The random potential problem leads to one of the simplest of those actions.

It comes down to the question of whether there are good techniques for evaluating this type of P.I. The most striking indication that really new results can be obtained was Feynman's polaron theory. He used a quadratic two-time action to define a soluble model or unperturbed problem. The difference between the actual action and the quadratic was taken as the perturbation. The choice of a model action is usually made on grounds of mathematical simplicity. One can also motivate the choice on physical grounds. Consider the particle to be coupled in a simple manner to a model dynamical system or reservoir. The model system can have fewer or more degrees of freedom than the original system that is coupled to the particle. It may be possible to eliminate the model system degrees of freedom and one is left with a model action for the averaged density matrix as a starting point for further analysis. As was the case for the P.I. approach to the potential problem, this can be combined with upper bound (U.B.) and lower bound (L.B.) techniques to obtain results outside the framework of conventional Hamiltonian approximation schemes.

To return to the Gaussian random potential, there are a number of questions that should be answered. First there is the dependence of ρ on g and β in the four limiting cases where one of the two variables is sent to either zero or infinity, with the other variable held fixed. What is the analytic dependence on dimensionality and on the type of covariance function $f(x)$? A second question is whether one can devise approximations to compute ρ to, say, a guaranteed accuracy of 1% for all values of g and β. A third question is to understand the analytic properties of ρ as a function of g and β. One might be able to answer the first two questions satisfactorily, without much insight into the third question. Even though there have been numerous studies, there is no systematic analysis of these questions. Our aim is to provide such analysis.

The average over the potentials that leads to the two-time action involves counting the contribution from a large number of different configurations. The partition function has the simplifying feature that each configuration contributes with the same sign. There are shallow and deep isolated traps, nearly overlapping traps, etc. From the eigenfunction decomposition of the density matrix for each configuration, we know that there will be distinct effects from bound states. What remains after the averaging process is not clear. Still, since the bound state properties of shallow traps depend on the space dimensionality, one expects the two time P.I. to have analytic properties that depend on dimensionality. It is desirable to put the mathematical schemes for evaluating path integral in correspondence with the physics of traps.

There is another type of problem that is of conceptual interest. It is the study of the white noise limit.[7–9] In d dimensions we take

$$W(x) = V_0 \frac{1}{L^d} \frac{1}{\pi^{d/2}} \exp(-x^2/L^2) \tag{7}$$

and ask for the behavior as $L \to 0$. The smoothest possible covariance function is used in taking this limit. The results are only finite for $d = 1$. But the nature of the divergence for $d \geqslant 2$ is of interest. One wants to isolate all of the divergent terms as $L \to 0$. For $d \geqslant 3$ the degree of divergence indicated by perturbation theory is wrong, but an analysis using a quadratic trial action leads to a tabulation of the divergent terms. For $d = 2$ this theory predicts a perturbation theory divergence for $V_0\beta < 2\pi$ and a stronger divergence for $V_0\beta > 2\pi$. It is not certain that the exact answer has this character.

The main tools of the analysis of this paper were developed in two earlier papers on upper and lower bounds for Wiener integrals.[10,11] The exact result is squeezed between upper and lower bounds. We start with relatively elementary approaches and proceed to more sophisticated methods as the subtleties emerge.

In Section 2 lower and upper bounds based on the free action are discussed. In one set of bounds one needs the correlation functions associated with graphs of increasing complexity. We write

$$I(\beta) = (2\pi\beta)^{d/2} < 0|\rho(\beta)|0\rangle = \exp E \tag{8}$$

Using the Feynman variation principle one finds the lower bound

$$E \geqslant g^2 H_1(\beta) \tag{9}$$

where $H_1(\beta)$ involves a correlation function $K_0(z \mid \beta)$ and the covariance function $f(z)$. We also have the trivial upper bound $E \leqslant g^2\beta^2/2$. Using coupling constant integrations we find a series of improvements. We also describe the Symanzik double time upper bounds and their improvement by coupling constant integration. This puts us on the road to squeezing the exact result when g and β are small. We also discuss the single-time Symanzik upper bound. This involves a β dependent potential with the shape and range of the covariance function. It exhibits effects due to shallow and deep traps and a dependence on dimensionality in the $g \to 0$; $\beta \to 0$ limit. The implications for the white noise limit are also examined.

In Section 3 we discuss a lower bound based on a simple trap picture, using a self-consistent-field type of functional. This is accurate for the first two terms in the $g \to \infty$ or $\beta \to \infty$ limit. It exhibits the dependence on the covariance function and some dimension-dependent results in a particularly simple form. The functional is inapplicable in the $g \to 0$ or $\beta \to 0$ limit when the free action bound is superior. Together with the upper bounds of Section 2 it establishes the nature of the white noise limiting behavior for $d \geqslant 3$.

In Section 4 the lower bounds are studied with a quadratic trial action. This has already been used to study some aspects of the problem by Bezak[12] and particularly by Samathiyakanit.[13] It was also used by the present author.[14] It provides a reasonable, rough overall picture applicable in all limits for g and β. The present treatment is more complete and uncovers some new features.

In Section 5 we treat the white noise limit, comparing the results of the lower bound free action, trap functional, and quadratic action estimates. As already mentioned, the nature of the divergent terms is clear for $d \geqslant 3$ and for $V_0\beta > 2\pi$ when $d = 2$.

In action 6, the delicate $d = 2$ white noise limit is discussed. The formulas of the quadratic action theory show an interesting transition at $V_0\beta = 2\pi$ from a logarithmic to quadratic divergence. There is still a gap between upper and lower bounds for the $V_0\beta < 2\pi$ sector. More powerful upper and lower bounds may be needed to establish the exact behavior.

In the conclusion we indicate some improvements that are feasible and mention areas where a strengthening of the analytic tools is needed.

2. BOUNDS BASED ON THE FREE PARTICLE ACTION

The noninteracting particle density matrix is

$$\langle x_1|\rho_F(\beta)|x_2\rangle = \int_{x_2}^{x_1} D_\beta x = (2\pi\beta)^{-d/2}\exp\left[-(x_1 - x_2)^2/2\beta\right] \tag{10}$$

It will be useful to introduce

$$\Delta_\beta x = (2\pi\beta)^{d/2} D_\beta x, \qquad \int_0^0 \Delta_\beta x = 1 \tag{11}$$

We study

$$I(\beta) = (2\pi\beta)^{d/2}\langle 0|\rho(\beta)|0\rangle = \int_0^0 \Delta_1 x \exp(\lambda A) \tag{12}$$

Here

$$\begin{aligned}\lambda &= g^2\beta^2/2\\ A &= \int f\left(\sqrt{\beta}\, z\right)\hat{\Phi}(z)\, d\mathbf{z}\end{aligned} \tag{13}$$

and $\hat{\Phi}(z)$ is the correlation functional

$$\hat{\Phi}(z) = \int_0^1\int_0^1 \delta\left[x(u) - x(u') - z\right] du\, du' \tag{14}$$

The perturbation series is

$$I = \sum_{m=0}^{\infty} \frac{\lambda^m}{m!}\int_0^0 \Delta_1 x A^m \equiv \sum_{m=0}^{\infty}\frac{\lambda^m}{m!} A_m \tag{15}$$

We need the N point correlation functions

$$K_F(\mathbf{z}_1\,|\,\mathbf{z}_2|\ldots\mathbf{z}_n) = \int_0^0 D_1 x\, \hat{\Phi}(\mathbf{z}_1)\ldots\hat{\Phi}(\mathbf{z}_n) \tag{16}$$

$$\begin{aligned}A_1 &= \int f\left(\sqrt{\beta}\, z_1\right) K_F(z_1)\, \mathbf{d}z_1\\ A_2 &= \int\int f\left(\sqrt{\beta}\, z_1\right) f\left(\sqrt{\beta}\, z_2\right) K_F(\mathbf{z}_1\,|\,\mathbf{z}_2)\, d\mathbf{z}_1\, d\mathbf{z}_2\end{aligned} \tag{17}$$

The lowest-order correlation function can be written in terms of the free particle density matrices as

$$\begin{aligned}K_F(z) = 2(2\pi)^{d/2}\int &\langle \mathbf{0}|\rho_F(1-u_1)|\mathbf{y}_1\rangle\langle \mathbf{y}_1|\rho_F(u_1-u_2)|\mathbf{y}_2\rangle\\ &\times\langle \mathbf{y}_2|\rho_F(u_2)|\mathbf{0}\rangle\delta(\mathbf{y}_1-\mathbf{y}_2-\mathbf{z})\end{aligned} \tag{18}$$

where

$$\int(\cdots)\to\int_0^1 du_1\int_0^{u_1} du_2\int\int d\mathbf{y}_1\, d\mathbf{y}_2(\cdots)$$

The integrals over $\mathbf{y}_1$ and $\mathbf{y}_2$ and over one of the "time" variables may be performed. Then

$$K_F(d||z) = \left(\frac{2}{\pi}\right)^{d/2} \int_0^\infty dx\,(1+x^2)^{(d-3)/2} \exp\left[-2z^2(1+x^2)\right] \quad (19)$$

where the d dependence in K_F has been indicated.

There is the exact result

$$K_F(d+2||z) = -\frac{1}{2\pi}\frac{1}{|z|}\frac{\partial}{\partial|z|}\cdot K_F(d||z) \quad (20)$$

so that one only needs K_F for $d=1$ and $d=2$. For $d=1$

$$K_F(1||z) = \frac{\sqrt{\pi}}{2}\operatorname{erfc}\left(\sqrt{2}\,|z|\right) \quad (21)$$

This leads to the particularly simple form for $d=3$:

$$K_F(3||z) = \frac{1}{\pi}\frac{1}{|z|}\exp(-2z^2) \quad (22)$$

K_F is defined so that $\int K_F(z)\,d\mathbf{z} = 1$. The limiting behavior as $|z|\to 0$ is

$$K_F(1||0) = (\pi/2)^{1/2}, \qquad K_F(2||z) \to \ln(1/|z|) \quad (23)$$

and $K_F(d||z) \to |z|^{2-d}$, $d \geqslant 3$. For $|z| \to \infty$

$$K_F(d||z) \sim \frac{1}{|z|}\exp(-2z^2), \qquad \text{all } d, \text{ as } z\to\infty \quad (24)$$

We now list lower and upper bounds that only involve $K_F(z)$. The Feynman lower bound, accurate to order g^2, is

$$\ln I \geqslant \lambda A_1 \quad (25)$$

The trivial upper bound [based on $f(z) \leqslant f(0) = 1$] is

$$\ln I \leqslant \lambda \quad (26)$$

This bound actually gives the leading term as $g\to\infty$ for fixed β or $\beta\to\infty$ for fixed g.

As was shown in our earlier paper, coupling constant integration on the trivial bound yields

$$I \leqslant 1 + A_1(e^\lambda - 1) \quad (27)$$

This improved bound interpolates between the exact limits. It is, however, a crude interpolation. There is another U.B. that also interpolates, but involves the full $K_F(z)$, rather than just A_1. It is the double-time Symanzik bound

$$I \leqslant \int d\mathbf{z}\, K_F(z) \exp\left[\lambda f\left(\sqrt{\beta}\, z\right)\right] \quad (28)$$

Next, we reduce the uncertainty in the value of I by taking into account second-order diagrams. They are needed to evaluate $K_F(\mathbf{z}_1 \,|\, \mathbf{z}_2)$. One has to take account of the different time orderings.

Analytically,

$$\begin{aligned} K_F(\mathbf{z}_1 \,|\, \mathbf{z}_2) = \frac{(2\pi)^{d/2}}{3} \int \{ &\delta(\mathbf{y}_1 - \mathbf{y}_2 - \mathbf{z}_1)\delta(\mathbf{y}_3 - \mathbf{y}_4 - \mathbf{z}_2) \\ &+ \delta(\mathbf{y}_1 - \mathbf{y}_4 - \mathbf{z}_1)\delta(\mathbf{y}_2 - \mathbf{y}_3 - \mathbf{z}_2) \\ &+ \delta(\mathbf{y}_1 - \mathbf{y}_3 - \mathbf{z}_1)\delta(\mathbf{y}_2 - \mathbf{y}_4 - \mathbf{z}_2)\} \\ &\times \langle \mathbf{o} | \rho_F(1 - u_1) | \mathbf{y}_1 \rangle \langle \mathbf{y}_1 | \rho_F(u_1 - u_2) | \mathbf{y}_2 \rangle \langle \mathbf{y}_2 | \rho_F(u_2 - u_3) | \mathbf{y}_3 \rangle \\ &\times \langle \mathbf{y}_3 | \rho_F(u_3 - u_4) | \mathbf{y}_4 \rangle \langle \mathbf{y}_4 | \rho_F(u_4) | 0 \rangle \end{aligned} \tag{29}$$

where $\int(\cdots) \to \int_0^1 du_1 \int_0^{u_1} du_2 \int_0^{u_2} du_3 \int_0^{u_3} du_4 \int\int\int\int d\mathbf{y}_1\, d\mathbf{y}_2\, d\mathbf{y}_3\, d\mathbf{y}_4 (\cdots)$. This may be simplified using Fourier and Laplace transforms, but we will not use the explicit form in this paper.

Using a coupling constant integration, we can improve the elementary Feynman bound. One finds

$$I \geqslant 1 + \frac{A_1}{A_2}\left[\exp\left(\lambda \frac{A_2}{A_1}\right) - 1\right] \tag{30}$$

This result is accurate to order g^4, but again does not go to the correct $g \to \infty$ limit.

A second coupling constant integration on the trivial upper bound yields the g^4 accurate result

$$I \leqslant 1 + \lambda A_1 + A_2[e^{\lambda} - 1 - \lambda] \tag{31}$$

There are other U.B. that require a knowledge of the full $K_F(\mathbf{z}_1 \,|\, \mathbf{z}_2)$. A coupling constant integration on the Symanzik double-time bound yields

$$I(g \,|\, \beta) \leqslant 1 + \int\int d\mathbf{z}_1\, d\mathbf{z}_2\, K_F(\mathbf{z}_1 \,|\, \mathbf{z}_2) \frac{f(\sqrt{\beta}\, z_1)}{f(\sqrt{\beta}\, z_2)}\left[\exp\left(\lambda f(\sqrt{\beta}\, z_2)\right) - 1\right] \tag{32}$$

This is also accurate to g^4 and contains the $g \to \infty$ limit. Finally there is a two-center U.B.

$$I \leqslant \int\int d\mathbf{z}_1\, d\mathbf{z}_2\, K_F(\mathbf{z}_1 \,|\, \mathbf{z}_2) \exp\left[\frac{\lambda}{2}\left\{f(\sqrt{\beta}\, z_1) + f(\sqrt{\beta}\, z_2)\right\}\right] \tag{33}$$

This is not accurate to order g^4, although it has the $g \to \infty$ limit. Its importance is that it is the second of a series of bounds that converges to the exact result.

We now take stock. The perturbation expansion can, of course, be reorganized into a cumulant expansion,

$$\ln I = \lambda A_1 + \tfrac{1}{2}\lambda^2\left(A_2 - A_1^2\right) + \cdots \tag{34}$$

However, the domain of accuracy is unclear. Our rearrangements of the same diagrams into expressions that represent upper and lower bounds provide a control on the accuracy. For example, for $\beta \sim 1$ one can squeeze the result for I so that the bounds are within 1% of each other for $g^2 < 2$. To do the same thing for large values of g^2, one needs mainly to improve the lower bounds. This will be done in a later section.

Here we note that the next step in improving upper bounds leads to some qualitative new features even in the region $g \ll 1$. These features are related to the inclusion of configurations representing shallow traps leading to bound states. The Symanzik single-time U.B. is

$$I \leqslant (2\pi\beta)^{d/2} \int_0^0 D_\beta x \exp\left[\frac{g^2\beta}{2} \int_0^\beta f(x(u))\,du\right] \tag{35}$$

or

$$I \leqslant \int_0^0 \Delta_1 x \exp\left\{\lambda \int_0^1 f\left(\sqrt{\beta}\, x(u)\right) du\right\} \tag{36}$$

This is the density matrix for a particle that moves in a potential whose shape is that of the covariance function and is of unit range. It has a temperature-dependent strength $g^2\beta/2 = -\lambda$. It can be analyzed by standard methods based on the solution of the Bloch equation. This was done explicitly for delta shell potential in Ref. 10.

There is a decisive dependence on dimensionality, even in the limit $g \ll 1$. For $d \geqslant 3$ there is no bound state. It makes an appearance only at a critical finite value of g that depends on β. On the other hand, for $d = 2$, there is at least one bound state for all values of g. When $g \ll 1$, I has a nonanalytic expansion of finite order. Thus, even if the upper and lower bounds of the first part of this section control I for $g \ll 1$, the physics of the shallow traps is missing.

The single-time Symanzik U.B. sheds light on some other points. It could be analyzed by approximation methods similar to those involving the quadratic, translation-invariant action, which we will apply later to the original I. For example, one can use the simple oscillator trial $-(\omega^2/2)\int_0^1 x^2\,du$ and determine $\omega(g, \beta)$. Then one does cumulant perturbation theory or upper- and lower-bound analysis. One finds that these methods are not adequate to deal with the weak bound state in two dimensions. The trial action must be more closely related to the shape of the covariance function $f(x)$.

It is easy to analyze the Symanzik U.B. in the limit $g \to \infty$ or $\beta \to \infty$ using an oscillator trial action. For the covariance $f(x) = \exp(-x^2)$ we find to leading order

$$\begin{gathered} \omega^2 \to g^2\beta^3/2 \\ \ln I \leqslant \frac{g^2\beta^2}{2} - \frac{d}{2}\omega + \frac{d}{2}\ln\omega + \cdots \end{gathered} \tag{37}$$

The first term coincides with the lower bound that is found from the trap functional (Section 3) or from a translation-invariant quadratic action (Section 4). The second term, corresponding to a harmonic well zero-point energy, however, has a coefficient that is smaller in magnitude than the corresponding lower-bound term. Thus the Symanzik U.B. is not as strong as we would like. Our multicenter generalizations[10] do not correct the second term to any finite order.

We now discuss the implications of the U.B. for the white noise limit. One can write

$$I \leqslant (2\pi\beta_0)^{d/2} \int_0^0 D_{\beta_0}x \exp\left\{ \frac{V_0 \beta L^{2-d}}{2\pi^{d/2}} \int_0^{\beta_0} \exp\left[-x^2(u) \right] du \right\} \tag{38}$$

Now as $L \to 0$, $\beta_0 = \beta/L^2 \to \infty$. In two dimensions, there is a contribution from the bound state eigenvalue which as a function of $V_0\beta/2\pi$. The corresponding contribution to $\ln I$ is β_0 times this function. Thus there is an L^{-2} divergence for all values of $V_0\beta/2\pi$. The gap between the upper and lower bounds is now very serious, since the harmonic lower bound yields only a logarithmic divergence.

3. SINGLE-TRAP LOWER BOUND

There is an elementary bound that is relevant to the $g \to \infty$ or $\beta \to \infty$ limits. Physically it describes the contributions of isolated deep traps to the partition function. This type of expression occurs in the collective variable theories of Halperin and Lax[15] and Zittarz and Langer.[16] A particularly simple result has been derived by Luttinger.[17] As applied to the Gaussian noise problem his variational method yields the lower bound

$$\begin{gathered} \ln I \geqslant E \\ E/\beta = -\frac{1}{2}\int \left(\frac{\partial \Psi}{\partial x} \right)^2 d\mathbf{x} + \int\int \frac{\beta}{2} \Psi^2(\mathbf{x}_1) W(\mathbf{x}_1 - \mathbf{x}_2) \Psi^2(\mathbf{x}_2)\, d\mathbf{x}_1\, d\mathbf{x}_2 \end{gathered} \tag{39}$$

Here Ψ is a normalized function chosen so as to maximize E. We refer to this expression as the trap functional. Donsker and Varadhan have established the remarkable result[18] that this gives the exact leading term as $\beta \to \infty$. They derive an upper bound which coincides with the lower bound. It leads to the nonlinear eigenvalue problem

$$-\tfrac{1}{2}\nabla^2\Psi - \beta\Psi(\mathbf{x})\int W(\mathbf{x}-\mathbf{x}_1)\Psi^2(\mathbf{x}_1)\,d\mathbf{x}_1 = \mu\Psi(\mathbf{x}) \tag{40}$$

It is possible to find the exact solution when $W(x)$ is a one-dimensional δ function. Our interest initially is in the case where the covariance length L is finite and is set equal to unity. The results depend primarily on a scale length b, the secondary dependence on the shape of Ψ. Let

$$\Psi(\mathbf{x}) = (b^{-d/2})\Psi_1(\mathbf{x}/b), \qquad \int \Psi_1^2\,d\mathbf{y} = 1 \tag{41}$$

$$\frac{E}{\beta} = -\frac{1}{2b^2}\int\left(\frac{\partial\Psi_1}{\partial y}\right)^2 dy + \frac{\beta g^2}{2}\int M(\mathbf{y})f(\mathbf{y}b)\,d\mathbf{y} \tag{42}$$

$$M(\mathbf{y}) = \int \Psi_1^2(\mathbf{y}-\mathbf{y}_1)\Psi_1^2(\mathbf{y}_1)\,d\mathbf{y}_1$$

dependence on β and g when $f(z) = \theta\,(1-|z|)$ or is a δ shell potential.

As βg^2 decreases, the size of the trap increases. To study the limit $\beta g^2 \ll 1$, consider the case of trial functions $\psi_1(y)$ such that $M(0)$, $M^1(0), \ldots$ are finite. Then as $b \to \infty$

$$\frac{E}{\beta} = -\frac{1}{2b^2}\int\left(\frac{\partial\Psi_1}{\partial y}\right)^2 dy$$

$$+\frac{\beta g^2}{2}\left\{\frac{M(0)}{b^d}\int f(\mathbf{y})\,d\mathbf{y} + \frac{M^1(0)}{b^{d+1}}\int |y| f\,d\mathbf{y} + \cdots\right\} \tag{43}$$

There is now a dependence on dimension. For $d = 1$, a solution with a localized solution and positive E is possible when $\beta g^2 \ll 1$. For $d \geqslant 3$ there is no solution when $\beta g^2 \ll 1$.

An overview of the content of the trap functional is possible with the function:

$$\Psi_1(x) = \left(\frac{2}{\pi}\right)^{d/4}\exp(-x^2) \tag{44}$$

The results are closely related to the leading terms of the first cumulant quadratic action lower bound. Then

$$\begin{aligned} M(x) &= (\pi)^{-d/2}\exp(-x^2) \\ E_d &= -\frac{\beta d}{2b^2} + \frac{g^2\beta^2}{2}(\pi)^{-d/2}\int f(yb)e^{-y^2}\,d\mathbf{y} \end{aligned} \tag{45}$$

For the function $f(z) = \exp(-z^2)$,

$$E_d = -\frac{\beta d}{2b^2} + \frac{g^2\beta^2}{2}(1+b^2)^{-d/2}$$
$$\frac{2}{g^2\beta} = b^4/(1+b^2)^{(-d/2-1)} \tag{46}$$

The explicit result for $d = 2$ is

$$E_2/\beta = \frac{g^2\beta}{2} - \sqrt{2}\, g\beta^{1/2} + 1$$
$$b^2 = \left(\frac{2}{g^2\beta}\right)^{1/2} \Big/ \left[1 - \left(\frac{2}{g^2\beta}\right)^{1/2}\right] \tag{47}$$

The size of the trap grows indefinitely as $g^2\beta \to 2$. We then switch to a delocalized solution and $E_2 = 0$ for $g^2\beta < 2$.

For $d \geqslant 3$ the localized solution is lost when $g^2\beta/2$ is of the order of unity. The switch to the extended solution occurs abruptly at a finite value of b.

For $d = 1$ the result for $g^2\beta/2 \ll 1$ is $b \to 2/g^2\beta \to \infty$ and $E_1 = \beta(g^2\beta/2)^2$. In this case the trap functional can be used for all values of $g^2\beta$. However, it is inferior to the free action bound in the $g \to 0$ limit.

We now discuss the predictions of the trap functional when the covariance length $L \to 0$. In one dimension there is a covergent result for E. The functional

$$\frac{E}{\beta} = -\frac{1}{2}\int\left(\frac{\partial\Psi}{\partial x}\right)^2 dx + \frac{\beta V_0}{2}\int \Psi^4\, dx \tag{48}$$

is maximized by

$$\Psi = \frac{(\beta V_0)^{1/2}}{2}\operatorname{sech}\left(x\frac{\beta V_0}{2}\right), \qquad E = \frac{\beta^3 V_0^2}{24} \tag{49}$$

In two dimensions, we introduce

$$\Psi(x)\frac{1}{(\gamma L)^{1/2}}\Psi_1\left(\frac{x}{\gamma L}\right)$$
$$E\cdot\frac{L^2}{\beta} = \frac{1}{2\gamma^2}\int\left(\frac{\partial\Psi_1}{\partial x}\right)^2 d^2x + \frac{\beta V_0}{2\pi}\int e^{-x^2\gamma^2} M(\mathbf{x})\, d^2x \tag{50}$$

This may be analyzed in the harmonic approximation. We find

$$\begin{aligned} \gamma^2 &= \left(\frac{2\pi}{\beta V_0}\right)^{1/2} \Big/ \left[1 - \left(\frac{2\pi}{\beta V_0}\right)^{1/2}\right] \\ E &= \frac{\beta}{L^2}\left\{\left(\frac{\beta V_0}{2\pi}\right)^{1/2} - 1\right\}^2 \end{aligned} \tag{51}$$

The leading divergent term agrees with the trivial U.B. $\gamma \to \infty$ as $\beta V_0/2\pi \to 1$ and we shift to an extended state with $E = 0$ when $\beta V_0/2\pi \leqslant 1$. We have examined a wide class of more accurate Ψ and find that the shift occurs at a somewhat lower value of βV_0, but there is still only a delocalized solution when $\beta V_0 \ll 1$. (However, we do not have a rigorous proof of this statement for the most general Ψ.) Thus, in two dimensions the trap functional has the remarkable feature that the divergence has a $1/L^2$ behavior when $\beta V_0 > 2\pi$ and $E = 0$ for $\beta V_0 \ll 1$. We know from the free action lower bound that the behavior of E is at least $\ln L$ in the latter case.

For $d \geqslant 3$ the leading term in E is $\beta V_0/(2\pi^{d/2}L^d)$ and an analysis by Taylor expansion of the covariance function is feasible. If Ψ is scaled by a length a we find in harmonic approximation that

$$a \sim L^{(d-2)/4}$$

The second term in E is $\sim 1/L^{(d/2)+1}$ and the third term is $1/L$. We find E as an expansion in a^2 and can write down the divergent terms. One needs $(4/d - 2)$ terms beyond the third term to reach the last serving term L^0. This analysis applies for any finite values of β and V_0.

4. QUADRATIC ACTION LOWER BOUND

We now work out the consequences of the lower-bound theory that uses a quadratic action. It is appropriate to both the $\beta \to \infty$, $g \to \infty$ limits, where it makes contact with the trap functional. It also goes over to the free action lower bound as $g \to 0$ or $\beta \to 0$.

Write

$$I = \int_0^0 \Delta_1 x \exp(\omega^2 A_0) \cdot \exp(\lambda A - \omega^2 A_0) \tag{52}$$

where A_0 is the quadratic form:

$$\begin{aligned} -A_0 &= \int_0^1 \int_0^1 \left[x(u) - x(u^1)\right]^2 du\, du^1 \\ A_0 &= -2\int_0^1 x^2\, du + 2\left(\int_0^1 x\, du\right)^2 \end{aligned} \tag{53}$$

The lower bound is

$$\ln I \geqslant \ln Q_0 - \omega^2 \frac{\partial \ln Q_0}{\partial(\omega^2)} + \langle A \rangle_0 \tag{54}$$

where

$$\begin{aligned} Q_0 &= \int_0^0 \Delta_1 x \exp(\omega^2 A_0) \\ \langle A \rangle_0 &= \frac{1}{Q_0} \int_0^0 \Delta_1 x\, A \exp(\omega^2 A_0) \end{aligned} \tag{55}$$

Here ω is to be chosen to make I as large as possible. One needs correlation functions for the "action" A_0. The second term in A_0 is handled by using the parametric identity

$$\exp(z^2/2) = (2\pi)^{-d/2} \int d\boldsymbol{\alpha} \exp\left(\boldsymbol{\alpha} \cdot \mathbf{z} - \frac{\alpha^2}{2}\right) \tag{56}$$

Let

$$\langle \mathbf{z} | r(1) | 0 \rangle = \int_0^z \Delta_1 x \exp(\omega^2 A_0), \qquad \omega = \Omega/2 \tag{57}$$

Then

$$\langle \mathbf{z} | r(1) | 0 \rangle = \Omega^d \int d\boldsymbol{\alpha}\, \langle \mathbf{z} + \boldsymbol{\alpha} | p(1) \boldsymbol{\alpha} | \rangle \tag{58}$$

where p is the density matrix for an oscillator of frequency Ω

$$\begin{aligned} \langle \mathbf{x}_1 | p(u) | \mathbf{x}_2 \rangle = &\left(\frac{\Omega}{\sinh \Omega u} \right)^{d/2} (2\pi)^{-d/2} \\ &\times \exp\left\{ \Omega \left[(\operatorname{csch} \Omega u) \mathbf{x}_1 \mathbf{x}_2 - (\coth \Omega u) \left(\frac{x_1^2 + x_2^2}{2} \right) \right] \right\} \end{aligned} \tag{59}$$

We have the explicit form[13,14,19]

$$\langle \mathbf{z} | r(1) | 0 \rangle = \left(\frac{\omega}{\sinh \omega} \right)^d \exp\left[-\frac{z^2}{2} \omega \coth \omega \right] \tag{60}$$

When $\omega \to 0$ the spatial range is 1. When $\omega \gg 1$ it is $1/\sqrt{\omega}$, describing a more localized state.

Using the identity and the standard rules for path integrals

$$\begin{aligned} &\int_0^z \Delta_1 x e^{\omega^2 A_0} \delta(\mathbf{x}(u_1) - \mathbf{y}_1) \\ &\quad = \Omega^d \int d\boldsymbol{\alpha}\, \langle \mathbf{z} + \boldsymbol{\alpha} | p(1 - u_1) | \mathbf{y}_1 + \boldsymbol{\alpha} \rangle \langle \mathbf{y}_1 + \boldsymbol{\alpha} | p(u_1) | \boldsymbol{\alpha} \rangle \end{aligned} \tag{61}$$

The translation-invariant form of A_0 gives rise to the α integration. The two-point function is

$$\int_0^z \Delta_1 x e^{\omega^2 A_0} \delta(\mathbf{x}(u_1) - \mathbf{y}_1)\delta(\mathbf{x}(u_2 - \mathbf{y}_2)$$
$$= \Omega^d \int d\alpha \langle \boldsymbol{\alpha} + \mathbf{z}|p(1-u_1)|\mathbf{y}_1 + \boldsymbol{\alpha}\rangle\langle \mathbf{y}_1 + \boldsymbol{\alpha}|p(u_1 - u_2)|\mathbf{y}_2 + \boldsymbol{\alpha}\rangle$$
$$\times \langle \mathbf{y}_2 + \boldsymbol{\alpha}|p(u_2)|\mathbf{a}\rangle \tag{62}$$

The correlation function that enters into the determination of the partition function is

$$K(z\,|\,\omega) \equiv \frac{1}{Q_0}\int_0^0 \Delta_1 x \int_0^1\int_0^1 \delta(\mathbf{x}(u) - \mathbf{x}(u_1) - \mathbf{z})\, du\, du'\, e^{\omega^2 A_0}$$
$$Q_0 = (\omega/\sinh\omega)^{d/2} \tag{63}$$

We find

$$K(d\,|\,|z|\omega) = \int_0^1 dv\,(2\pi H)^{-d/2}\exp(-z^2/2H)$$
$$H = (\cosh\omega - \cosh\omega v)/2\omega\sinh\omega \tag{64}$$

We have $\int K(\alpha\,|\,|z|\omega)\, d\mathbf{z} = 1$. The relation between the K for different dimensions is

$$K(d+2\,|\,|z|\omega) = -\frac{1}{2\pi}\frac{1}{|z|}\frac{\partial}{\partial|z|}K(d\,|\,|z|\omega) \tag{65}$$

The lower bound is

$$\ln I \geqslant \to T + \frac{g^2\beta^2}{2}\int \Phi(z)\int_0^1 dv\, f\left[|z|(2\beta H)^{1/2}\right] dz \tag{66}$$

where

$$T \equiv \ln Q_0 - \frac{\omega^2 \partial \ln Q_0}{2(\omega^2)} = -d\ln\left(\frac{\sinh\omega}{\omega}\right) - \frac{d}{2}(1-\coth\omega) \tag{67}$$

We can obtain explicit results in the limiting cases: low frequency, $\omega \ll 1$; high frequency, $\omega \gg 1$. What this means in terms of the parameters g and β emerges from the analysis. The intermediate case can be analyzed numerically by plotting $g(\beta,\omega)$ from $\partial \ln I/\partial\omega = 0$, and inverting graphically.

We study three types of correlation function: (a) $f(z) = \delta(z)$ in one dimension, (b) $f(z) = \exp(-|z|)$, (c) $f(z) = \exp(-z^2)$.

4.1. Low-Frequency Limit

We will obtain an improvement on the lower bound provided by the free action. However, the result is not completely accurate to order g^4. To obtain this one needs a lower bound based on a coupling constant integration. This is not done in this paper.

For $\omega \ll 1$,

$$\begin{aligned} T &\to -\frac{d}{180}\omega^4 \\ H &\to \frac{1}{4}(1-u^2)\left[1-(1-u^2)\frac{\omega^2}{12}+\cdots\right) \end{aligned} \tag{68}$$

In all cases the optimum frequency ω is proportional to g.

In the one-dimensional δ-function case,

$$\langle A\rangle_0 \to \frac{g^2\beta^{3/2}}{2}\left(\frac{\pi}{2}\right)^{1/2}\left(1+\frac{\omega^2}{48}+\cdots\right) \tag{69}$$

$$\begin{aligned} \omega^2 &\to \frac{15}{16}\left(\frac{\pi}{2}\right)^{1/2} g^2\beta^{3/2} \\ E &\to \left(\frac{\pi}{2}\right)^{1/2}\frac{g^2\beta^{3/2}}{2}+\frac{1}{180}\omega^4 \end{aligned} \tag{70}$$

The expansion requires $g^2\beta^{3/2} \ll 1$.

For more general $f(z)$, with $\Phi(z) = e^{-z^2}/\pi^{d/2}$,

$$\begin{aligned} \langle A\rangle_0 = \frac{g^2\beta^2}{2}\Bigg\{&\int d\mathbf{z}\,\Phi(z)\int_0^{\pi/2}(\sin\theta)f\left[\left(\frac{\beta}{2}\right)^{1/2}|z|\sin\theta\right]d\theta \\ &-\frac{\omega^2}{24}\left(\frac{\beta}{2}\right)^{1/2}\int d\mathbf{z}\,\Phi(z)|z| \\ &\times\int_0^{\pi/2}(\sin^4\theta)f^1\left[\left(\frac{\beta}{2}\right)^{1/2}|z|\sin\theta\right]\Bigg\}\,d\theta \end{aligned} \tag{71}$$

$$\omega^2 = -\frac{90}{d}\frac{g^2\beta^2}{48}\left(\frac{\beta}{2}\right)^{1/2}\int d\mathbf{z}\,\Phi(z)\int_0^{\pi/2}\sin^4 lf^1\left[\left(\frac{\beta}{2}\right)^{1/2}|z|\sin\theta\right]d\theta \tag{72}$$

The increase in E is $(d/180)\omega^4$.

For $f(z) = e^{-|z|}$ we have as $\beta \to 0$, $\omega^2 \to g^2\beta^{5/2}$, while for $f(z) = e^{-z^2}\omega^2 \to g^2\beta^3$. If $g \ll 1$, ω becomes large as $\beta \to \infty$ for dimensionality less or equal to three.

4.2. High-Frequency Theory

In the high-frequency limit we neglect all exponential contributions of type $e^{-\omega}$. Then

$$T \to -\frac{d\omega}{2} + d\ln\omega - \frac{d}{2}$$
$$H \to \frac{1}{2\omega}\left(1 - e^{-\omega(1-u)}\right) \tag{73}$$

In the extreme $\omega \gg 1$ limit we take $H \to 1/2\omega$ and neglect the $d\ln\omega$ and $-d/2$ terms in T. We define a parameter

$$x = (\beta/\omega)^{1/2} \tag{74}$$

E becomes the trap function with Gaussian trial and with x identified with the length b of Eq. (41). x must be less than 1 for the validity of the high-frequency expansion.

Our aim is now to obtain all of the surviving terms in E as $g \to \infty$ (fixed β) and as $\beta \to \infty$ (fixed g). We start with the one-dimensional δ function where the main features of the calculation emerge in a simple way.

4.2.1. One-Dimensional δ Function. The result, neglecting exponential terms, is explicitly

$$\langle A\rangle_0 = \frac{g^2\beta^2}{2}\frac{1}{\sqrt{\pi}}\frac{1}{x}\left[1 + \frac{1}{\beta}x^2\left(\frac{\pi}{2} - \ln 2\right)\right] \tag{75}$$

Define the expansion parameter

$$\delta = \frac{2\sqrt{\pi}}{g^2\beta} \tag{76}$$

Then

$$E = \ln(2\beta) - \frac{1}{2} - \frac{\beta}{2x^2} + \frac{\beta}{\delta x} + \frac{x}{\delta}\left(\frac{\pi}{2} - \ln 2\right) - 2\ln x \tag{77}$$

The condition $\partial E/\partial x = 0$ yields

$$\delta\left(1 - \frac{2x^2}{\beta}\right) = x - \frac{x^3}{\beta}\left(\frac{\pi}{2} - \ln 2\right) \tag{78}$$

Using this to eliminate the $-\beta/2x^2$ term,

$$E = \frac{\beta}{2\delta^2} + \ln(2\beta) - \frac{3}{2} - 2\ln x + \frac{x}{\delta}\left[1 + \frac{3}{2}\left(\frac{\pi}{2} - \ln 2\right)\right]\frac{x^2}{2\delta}\left(\frac{\pi}{2} - \ln 2\right) \tag{79}$$

We find an expansion

$$x = \delta + \frac{\delta^3}{\beta}\left(\frac{\pi}{2} - \ln 2 - 2\right) + \cdots \tag{80}$$

For the surviving terms as $g \to \infty$ or $\beta \to \infty$ we only need $x \approx \delta$ in Eq. (82). Then

$$\begin{aligned} &\omega \to g^4\beta^3/4\pi \\ &E \to \frac{\beta}{2\delta^2} + \ln 2\beta - 2\ln\delta - \frac{1}{2} + \frac{3}{2}\left(\frac{\pi}{2} - \ln 2\right) \end{aligned} \tag{81}$$

We have the conditions $g^2\beta > 2\sqrt{\pi}$ and $g^2\beta \cdot \beta^{1/2} > 2(2\pi)^{1/2}$. Since the lead term is only equivalent to the Gaussian trial function in the trap functional we have $E \to g^4\beta^3/8\pi$ instead of the exact $g^4\beta^3/24$.

To treat more general covariance functions in the high-frequency limit, write the average of the action as

$$\langle A \rangle_0 = \frac{g^2\beta^2}{2}\int\int_0^1 d\eta\, f\left[|z|x(1 - e^{-\omega\eta})^{1/2}\right]\Phi(z)\, d\mathbf{z} \tag{82}$$

Consistent with the neglect of exponential contributions, this may be put in the form

$$\begin{aligned} \langle A \rangle_0 = {} & \frac{g^2\beta^2}{2} + \frac{g^2\beta^2}{2}\int \Phi(z)\left[f(|z|x) - 1\right] d\mathbf{z} \\ & + \frac{g^2\beta}{2}x^2\int_0^1 d\eta \int d\mathbf{z}\, \Phi(z)\left\{f\left[|z|x(1 - e^{-\eta})^{1/2}\right] - f(|z|x)\right\} \end{aligned} \tag{83}$$

$$T = -\frac{d\beta}{2x^2} - 2d\ln x + d\ln(2\beta) - d/2 \tag{84}$$

4.2.2. $f(z) = \exp(-|z|)$. Using this to eliminate the $-\beta/2x^2$ term,

$$E = \frac{\beta}{2\delta^2} + \ln(2\beta) - \frac{3}{2} - 2\ln x + \frac{x}{\delta}\left[1 + \frac{3}{2}\left(\frac{\pi}{2} - \ln 2\right)\right]\frac{x^2}{2\delta}\left(\frac{\pi}{2} - \ln 2\right) \tag{85}$$

We find an expansion

$$x = \delta + \frac{\delta^3}{\beta}\left(\frac{\pi}{2} - \ln 2 - 2\right) + \cdots \tag{86}$$

We define

$$\Lambda_m \equiv \int |z|^m \Phi(z)\, d\mathbf{z} \tag{87}$$

$$\begin{aligned} F(x) &= \frac{1}{\Lambda}\int \Phi(z)\, d\mathbf{z}\,(e^{-|z|x}-1) \\ &= -x + \sum_{n=2}^{\infty} F_n x^n/n! \end{aligned} \tag{88}$$

$$\begin{aligned} G(x) &= \frac{x^2}{\Lambda_1}\int_0^{\infty} d\eta \int d\mathbf{z}\,\Phi(z)\Big[\exp\big(-|z|x(1-e^{-\eta})^{1/2} - \exp(-|z|x)\Big] \\ &\equiv \sum_{n=3}^{\infty} G_n x^n/n! \end{aligned} \tag{89}$$

A useful expansion parameter is

$$\gamma^3 = 2\alpha/g^2\beta\Lambda_1 \tag{90}$$

Then

$$\begin{aligned} E &= \frac{g^2\beta^2}{2} + d\ln(2\beta) - \frac{d}{2} + \Delta E \\ \Delta E &= \frac{d\beta}{2x^2} - 2d\ln x + \frac{d\beta}{\gamma^3}\left[F + \frac{1}{\beta}G\right] \end{aligned} \tag{91}$$

The condition $\partial E/\partial x = 0$ yields

$$\gamma^3 = -x^3(F^1 + G^1/\beta)/(1-2x^2/\beta) \tag{92}$$

As in the one-dimensional δ function case, we use this to write

$$\Delta E = -2d\ln x + \frac{d\beta}{\gamma^3}\left\{F + G + \frac{x}{2}\,\frac{F^1 + G^1/\beta}{1-2x^2/\beta}\right\} \tag{93}$$

We can now set about to determining all the terms in ΔE that survive when $g \to \infty$ or $\beta \to \infty$.

One only needs x to lowest order ($x \to \infty$) in the following terms:

$$\begin{aligned} &\frac{d}{\gamma^3}\left(G + x\frac{G^1}{2}\right) \to 5d(1-\ln 2) \\ &\frac{d}{\gamma^3}x^3F^1 \to d \end{aligned} \tag{94}$$

Thus all of the surviving terms are contained in

$$\Delta E = -2d\ln\gamma + \big[5(1-\ln 2) - 1\big]d + \frac{d\beta}{\gamma^3}\left\{F + \frac{x}{2}F^1\right\} \tag{95}$$

The leading term is $-(3/2)d\beta x/\gamma^3$, so that we require x to an accuracy of γ^3 and γ^3/β.

Let $\xi(\gamma)$ be the solution of

$$\gamma^3 = -\xi^3 F^1(\xi) \tag{96}$$

expressed as a series

$$\xi = \sum c_n \gamma^n, \qquad c_1 = 1 \tag{97}$$

Then

$$x = \xi(\gamma) + \frac{\gamma^3}{\beta}\left[\frac{2}{3}F_2 + 2(1 - \ln 2) - \frac{2}{3}\right] \tag{98}$$

Finally,

$$\Delta E = -2d\ln\gamma + \alpha\left[2(1-\ln 2) - F_2\right] + \frac{d\beta}{\gamma^3}\left(F + \frac{\xi}{2}\frac{dF}{d\xi}\right) \tag{99}$$

This completes the task of finding the surviving terms for the covariance function $f(z) = \exp(-|z|)$. The leading term is $x \to \infty$ or

$$\omega \to g^{4/3}\beta^{5/3}\left(\frac{\Lambda_1}{2d}\right)^{2/3} \tag{100}$$

We require $g^2\beta > 1$ and $g^2\beta \cdot \beta^{3/2} > 1$.

4.2.3. $f(z) = e^{-z^2}$. For this covariance function choose

$$F(x) = \frac{1}{d}\left\{(1+x^2)^{-d/2} - 1\right\} \tag{101}$$

$$G(x) = \frac{1}{d}\,\frac{x^2}{(1+x^2)^{d/2}}\int_0^\infty d\eta\left\{\left(1 - \frac{x^2}{1+x^2}e^{-\eta}\right)^{-d/2} - 1\right\} \tag{102}$$

We now have $F^1(x\to 0) \to -x$, $F(x \to 0) \to -x^2/2$.

Equations (90)–(93) now apply with γ^3 replaced by $2/g^2\beta$. In addition the expansions are in even powers of x. The study of the surviving terms requires minor modifications. We find

$$\Delta E = -\frac{d}{2}\ln\left(\frac{2}{g^2\beta} + \frac{d}{2} + d\beta\left(\frac{2}{g^2\beta}\right)\left(F + \frac{x}{2}F^1\right)\right. \tag{103}$$

To requisite accuracy,

$$x = \xi - \left(\frac{d+1}{2}\right)\frac{1}{2\beta}\left(\frac{2}{g^2\beta}\right)^{3/4} \tag{104}$$

where ξ is the solution of

$$\frac{2}{g^2\beta} = -\xi^3 \frac{dF}{d\xi} \tag{105}$$

In leading order $\xi \sim (2/g^2\beta)^{1/4}$. The series then goes in steps of $(2/g^2\beta)^{1/2}$. For the covariance function $f = \exp(-z^2)$ the leading term for the frequency is $\omega \to g\beta^{3/2}/\sqrt{2}$. This has the same dependence on g and β as for the low-frequency case, but with a different coefficient.

It should not be forgotten that the coefficients of the divergent terms will be changed when one computes the second- and third-order cumulants. However, the nature of the series is unaltered.

5. THE WHITE NOISE LIMIT

We now adapt our results to study the behavior of the partition function as the covariance length $L \to 0$. We approach this limit with the smooth covariance function

$$W(x) = \frac{V_0}{2L^d} \frac{\exp(-x^2/L^2)}{\pi^{d/2}} \tag{106}$$

In the one-dimensional case we have obtained finite results.

First note the behavior predicted by the free action lower bound. In two dimensions we have

$$\begin{aligned} E_2 &> \frac{\beta V_0}{4\pi} \frac{1}{q} \ln\left(\frac{q + 1/2}{q - 1/2} \right) \\ q^2 &= \frac{1}{4} + \frac{L^2}{2\beta} \end{aligned} \tag{107}$$

Thus there is a logarithmic divergence as $L \to 0$. We know that this is wrong when $V_0\beta/2\pi > 1$, since the trap functional gives a better lower bound which diverges as $1/L^2$. On the other hand, the trap functional with a Gaussian trial function leads to an infinitely extended state when $V_0\beta \ll 1$, implying only $E_2 \geqslant 0$. So the free action bound is superior. The two-dimensional case is particularly delicate, and we take up the analysis with the harmonic trial action in the next section. The question at issue is whether there is a change in the degree of divergence at a finite value of $V_0\beta$.

In three dimensions the free action lower bound is

$$E_3 \geqslant \frac{V_0\beta}{L} \pi^{3/2} \frac{1}{1 + 2L^2/\beta} \tag{108}$$

with a linear divergence as $L \to 0$. On the other hand the trap functional yields a lower bound

$$E_3 \geqslant \frac{\beta^2 V_0}{2\pi^{3/2}} \frac{1}{L^3} - 3\left(\frac{V_0 \beta^3}{8\pi^{3/2}} \right)^{1/2} 1/L^{5/2} \tag{109}$$

The leading term coincides with the trivial upper bound. So there is indeed a $1/L^3$ divergence. It only remains to find the surviving terms as $L \to 0$. The same holds true for $d \geqslant 4$ with coincidence of the leading terms in the U.B. and L.B.

For $d \geqslant 3$ one can find the set of divergent terms for the trap functional. The first two terms are exact. However, the coefficients of the subsequent terms are not exact, and we miss a $\ln L$ term. For the smooth covariance functional $L^{-d}\exp(-x^2/L^2)$, the quadratic action also gives the first two terms. In addition the logarithmic term is accurate.

A simple special case of the quadratic action lower bound is a bound based on $\exp(-x^2) \geqslant 1 - x^2$. We choose

$$\omega = \left(\frac{V_0}{8\pi^{d/2}} \right)^{1/2} \beta^{3/2} \Big/ L^{(1+d/2)} \tag{110}$$

It is then not necessary to evaluate a first cumulant. The lower bound is simply

$$E_d \geqslant -d \ln\left(\frac{\sinh \omega}{\omega} \right) + \frac{\beta^2}{L^d} \frac{V_0}{2\pi^{d/2}} \tag{111}$$

The first two terms are exact, as is the coefficient of the logarithmic term.

A more complete analysis with the quadratic action, including the improvement from the average of the residual action, may be carried out by adapting the results of Section 4. The number of divergent terms depends on the dimensionality. The expansion parameter is

$$\psi_0 = \left(\frac{2\pi}{V_0 \beta} \right)^{1/4} L^{(d-2/4)} \tag{112}$$

The series proceeds in powers of ψ_0^2. Thus the first term beyond the $-d\omega$ term is of order L^{-2}, and the term beyond that is of order $L^{(d/2-3)}$. It is the last surviving term if $d \geqslant 6$. For general d we must include $(d+2)/(d-2)$ terms beyond the $-d\omega$ term. While the degree of divergence of the most divergent term increases with the dimension, the number of divergent terms increases.

The theory of the $L \to 0$ is incomplete until we compute the corrections arising from a small number of higher cumulants. The number needed again depends on d. This changes the coefficients of the divergent terms, but the nature of the series is unaltered.

6. TWO-DIMENSIONAL CASE

We have found that the $L \to 0$ limit presents special problems in the two-dimensional case. We present the lower bound estimate provided by the quadratic trial action.

For the Gaussian covariance function, the explicit result is

$$\langle A \rangle_0 = \frac{V_0 \beta}{2\pi} \frac{\sinh \omega}{(\sigma^2 - 1)^{1/2}} \ln \left[\frac{\sigma \cosh \omega - 1 + (\sigma^2 - 1)^{1/2} \sinh \omega}{\sigma - \cosh \omega} \right] \tag{113}$$

$$\begin{gathered} \sigma = \cosh \omega + \frac{\omega}{\beta_0} \sinh \omega \\ \beta_0 \equiv \beta / L^2 \end{gathered} \tag{114}$$

We will also need the complete expression for T.

The key parameter is

$$\alpha = (V_0 \beta / 2\pi)^{1/2} \tag{115}$$

There are two domains depending on whether $\alpha > 1$ or $\alpha < 1$.

(1) $\alpha > 1$. As was noted earlier the high-frequency expansion $\omega \gg 1$ is relevant when $\alpha > 1$. Then $\omega \to \infty$ and

$$\frac{1}{x_0} = \left(\frac{\omega}{\beta_0} \right)^{1/2} = \left(\frac{\omega}{\beta} \right)^{1/2} L \tag{116}$$

is finite and nonzero as $L \to 0$. In this limit

$$\langle A \rangle_0 \to \alpha^2 \beta_0 (1 + x_0^2)^{-1} \left[1 + \frac{x_0^2}{\beta_0} \ln(1 + x_0^2) \right] \tag{117}$$

$$T \to 2 \ln(2\beta_0)^{-1} - \frac{\beta_0}{x_0^2} - 2 \ln x_0 \tag{118}$$

To order L^2

$$\frac{1}{x_0^2} = \alpha - 1 + \frac{\alpha x_0^4}{4\beta_0} \tag{119}$$

There is no solution of this equation for $\alpha \ll 1$. To order L^0

$$E = \beta_0 (\alpha - 1)^2 + 2 \ln(2\beta_0) - 1 + \alpha \ln\left(\frac{\alpha}{\alpha - 1} \right) + \ln(\alpha - 1) \tag{120}$$

There are both $1/L^2$ and $\ln(1/L)$ divergent terms

(2) $\alpha < 1$. Here the frequency ω is finite as $L \to 0$ and $1/x_0 \to 0$:

$$\langle A \rangle_0 \to \alpha^2 \ln(2\beta_0) + \alpha^2 \ln[(\sinh \omega)/\omega] \tag{121}$$

$$E \to \alpha^2 \ln(2\beta_0) + (\alpha^2 - 2) \ln[(\sinh \omega)/\omega] + \omega \coth \omega - 1 \tag{122}$$

The low-frequency theory is obtained when $\alpha \ll 1$. Then

$$\begin{aligned} \omega &\to \tfrac{1}{2}\sqrt{30}\,\alpha \\ E &\to \alpha^2 \ln(2\beta_0) + \tfrac{5}{8}\alpha^4 \end{aligned} \tag{123}$$

with a logarithmic divergence in L.

However, we can now do better and study the approach $\alpha \to 1$ with $\alpha < 1$. We have $\omega > 1$, but it is independent of L as $L \to 0$. Then

$$\begin{aligned} \omega &\to (2-\alpha^2)/(1-\alpha^2) \\ E &\to \alpha^2 \ln(2\beta_0) + (\alpha^2 - 2)\left[\omega - \ln(2\omega)\right] + \omega - 1 \end{aligned} \tag{124}$$

Now, as $\alpha \to 1$

$$\begin{aligned} \omega &\to \frac{1}{2}\,\frac{1}{(1-\alpha)} \\ E &\to \alpha^2 \ln(2\beta_0) + \ln\left(\frac{1}{1-\alpha}\right) - 2 \end{aligned} \tag{125}$$

This is the domain that cannot be handled by the trap bound or by the free action bound. The divergence is logarithmic. There we have the prediction of the quadratic action of a remarkable transition at $\alpha = 1$ from a logarithmic to a quadratic divergence.

The reality of this transition is at present uncertain. The analysis of the trap functional shows that the quadratic divergence persists to values of α somewhat less than 1. Our analysis of the case $\alpha \ll 1$ in Section 3 is incomplete. We found no trap for $\alpha \ll 1$ provided the trial function $\psi_1(x)$ is such that $M(0), M^1(0), \ldots$ exist. It may be that there is a trap with $E_2 \neq 0$, in which case the quadratically divergent lower bound would be established for all α. We have made a variational analysis of the two-dimensional trap functional, using trial functions of the type that yields the two-dimensional bound state for the potential problem. We find no localized solution when $\beta V_0 \ll 1$. However, a rigorous analysis of the trap functional is missing.

7. CONCLUSIONS

The path integral representing the averaged partition function for a particle subject to Gaussian random potentials is one of the simplest two-time integrals with nontrivial content. When the covariance length is finite the partition function depends on the strength g, the inverse temperature β, the dimensionality d, and on analytic properties of the covariance function. The partition function is a much simpler quantity than averages of products of Green's functions, since everything is real and positive. One can then apply upper- and lower-bound techniques. A series of improved bounds can be related both to the inclusion of different types of configuration and to systematic approximation schemes. It seems worthwhile to try to realize this in detail, and to make the mathematics corresponds to physical intuition.

When a problem is as simple as the present one, yet similar mathematically to many other problems, we would like to see it treated in depth. Existing approaches are rather piecemeal and we have tried to make a start on a more thorough study.

There are a number of points where our results are incomplete, but can be made complete in a relatively straightforward manner. One of these is the calculation, for the quadratic action, of the higher cumulant terms in the expansion as $g \to \infty$, $\beta \to \infty$, or $L \to 0$. Using coupling integrations, the correlation functions occurring in the higher cumulants can also be used to find better lower bounds. One coupling integration probably solves the problem of calculating the partition function to 1% accuracy. This will be done in sequel to the present paper.

A second point is to develop model actions which express the feature that the covariance function falls to zero at large distances. The quadratic action is unphysical in this respect. We have been able to find a systematic scheme of model actions that deal with this problem and provide improved lower bounds. It is however not easy to work with them. This will also be developed in the sequel. As noted in the body of the paper the single-time Symanzik upper bound and even the multipoint and coupling integration generalizations noted in Ref. 1 are not strong enough to close the gap between upper and lower bounds in a number of cases. Examples where there is a gap in the leading term are the upper bounds for the one-dimensional δ function and for the model quadratic action. The Donsker–Varadhan result shows that the lower-bound result is correct as $\beta \to \infty$. In other cases the coefficient of the second term of the upper-bound expansion is not correct. It might be possible to improve the upper bounds by using the Symanzik technique with suitable trial actions. But new ideas may be needed.

REFERENCES

1. R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
2. R. P. Feynman, *Statistical Mechanics* (W. A. Benjamin, Reading, Machusetts, 1972).
3. K. Symanzik, *J. Math. Phys.* **6**:1155 (1965); E. Lieb, *Bull. Am. Math. Soc.* **82**:751 (1976); L. W. Bruch, *J. Chem. Phys.* **55**:5101 (1971).
4. S. F. Edwards and V. B. Gulyaev, *Proc. Phys. Soc.* **83**:495 (1964); R. Jones and T. Lukes, *Proc. R. Soc. London Ser. A* **309**:457 (1969).
5. R. Friedberg and J. M. Luttinger, *Phys. Rev. B* **12**:4460 (1975).

6. E. P. Gross, *J. Math. Phys.* **24**:399 (1983).
7. D. J. Thouless, *J. Phys. C.* **9**:L603 (1976).
8. V. Sayakanit, *J. Phys. C.* **11**:L521 (1978).
9. A. B. Harris and T. C. Lubensky, *Phys. Rev. B* **23**:2640 (1981).
10. E. P. Gross, *J. Stat. Phys.* **30**:45 (1983).
11. E. P. Gross, *J. Stat. Phys.* **31**:115 (1983); **21**:215 (1979).
12. V. Bezak, *Proc. Phys. Soc. A* **315**:339 (1970); *J. Phys. A* **4**:324 (1971).
13. V. Samthiyakanit, *J. Phys. C* **7**:2849 (1974); V. Sa-yakanit, *Phys. Rev. B* **19**:2266 (1979); V. Sa-yakanit and H. R. Glyde, *Phys. Rev. B* **22**:6222 (1980).
14. E. P. Gross, *J. Stat. Phys.* **17**:265 (1977).
15. B. I. Halperin and M. Lax, *Phys. Rev.* **148**:722 (1966); **153**:802 (1967).
16. J. Zittarz and J. M. Langer, *Phys. Rev.* **148**:741 (1966).
17. J. M. Luttinger, *Phys. Rev. Lett.* **37**:609 (1976); *J. Math. Phys.* **23**:1011 (1982).
18. M. D. Donsker and S. R. S. Varadhan, in *Functional Integration and Its Application*, A. M. Arthurs, ed. (Oxford University Press, New York, 1975); cf. B. Simon, *Functional Integration and Quantum Physics* (Academic Press, New York, 1979).
19. G. J. Papadopoulos, *J. Phys. A* **7**:183 (1974).