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Functional Integral Representations of Partition Function Without Limiting Procedure. Techniques of Calculation of Moments

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A definition of the Feynman path integral which does not rest on a limiting procedure based on time-slicing has been given by DeWitt-Morette. We present in this paper a discussion of real Gaussian measures and formulate expressions for the quantum statistical partition function directly in terms of measures of integration on the topological vector space ϕ_0 of continuous functions defined on the time interval $T = (t_a, t_b)$, such that $x(t_a, t_b) = 0$ for all $x \in \phi_0$. We give a definition of a measure for the space ϕ_0 equivalent to the path integral based on the Uhlenbeck-Ornstein probability distribution. We give expressions for the partition function using the Wiener-Feynman measure and the Uhlenbeck-Ornstein measure. As an exercise in the use of the new techniques, we present calculations of moments of potential functions. The techniques will enable one to solve in a rigorous manner practical problems in quantum statistical mechanics.

KEY WORDS: Partition function; moments; Feynman measure; Uhlenbeck-Ornstein measure; topological vector space; path integral.

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1. INTRODUCTION

A definition of Feynman's path integral which does not rest on a limiting procedure, based on time-slicing, has been given recently by DeWitt.[1,2] This new development has provided the missing rigor to the path-integral formalism of quantum mechanics and quantum statistical mechanics. In the literature various measures for function space integration have been proposed. The two important measures are the Wiener–Feynman[3] and the Uhlenbeck–Ornstein[4,5] measure. The importance of the Uhlenbeck–Ornstein measure is in the path-integral formulation of quantum statistics, where it has been shown[4] that it results in a great improvement in the approximate evaluation of the partition function with decreasing temperature and/or decreasing relative magnitude of the anharmonic part of the potential.

The formalism proposed by DeWitt in Refs. 1 and 2 is valid for complex Gaussian measures and in that form is particularly suited for the study of problems in particle physics and especially for the study of gauge fields. We present extensions of DeWitt's results to real Gaussian measures[2] and formulate expressions for the partition function in terms of measures of integration on the topological vector space ϕ_0 of continuous functions defined on the time interval $T = (t_a, t_b)$ such that $x(t_a) = x(t_b) = 0$ for all $x \in \phi_0$. We state in Section 2 an immediate extension of propositions stated and proved in Refs. 1 and 2 for evaluating integrals over the function space ϕ_0, which we shall need for the approximate calculations of the partition function. In Section 3 we given an expression for the partition function using the Wiener–Feynman measure on the space ϕ_{xx}, which is the space of continuous paths x on T such that $x(t_a) = x(t_b) = x$. We calculate in that section moments of the potential function using the propositions stated in Section 2. In Section 4 we give a definition of measure for the space ϕ_0 equivalent to the path integral based on Uhlenbeck–Ornstein probability distributions and give an expression for the partition function using this measure on the space ϕ_{xx}. An an exercise in the use of the new techniques, we present calculations of moments of potentials. The examples covered in Sections 3 and 4 should familiarize the reader with the use of new, versatile techniques.

It may be emphasized that the final results obtained are not new and the spirit of this paper is no more than to present rigorous calculations of results contained in Refs. 3–5. The last section of this paper gives conclusions and directions in which further investigations may be pursued.

[2] We refer to as a measure on topological vector space what is called a promeasure in Refs. 1 and 2.

2. NOTATIONS AND PROPOSITIONS[3]

We consider a space ϕ_0 of continuous path x of uniform norm defined on a time interval $T = (t_a, t_b)$ such that

$$x(t_a) = x(t_b) = 0$$
$$\|x(t)\| = \sup|x(t)| \qquad \text{for} \quad t \in T$$

In the function space integral formulation of the quantum partition function one encounters integrals of a functional $\varphi(x)$ on ϕ_0, which may be written symbolically

$$\langle\varphi(x)\rangle_{\phi_0} = \int_{\phi_0} \varphi(x)\, d\omega(x) \tag{1}$$

where ω is the real Gaussian measure whose Fourier transform $F\omega$ is

$$F\omega(\mu) = \exp[-\tfrac{1}{2}W(\mu)] \tag{2}$$

$W(\mu)$ is a quadratic form on M, the dual of ϕ_0 defined by

$$W(\mu) = \int_T d\mu(r) \int_T d\mu(s)\, G(r, s) \tag{3}$$

M is the space of bounded measure μ on T such that

$$\langle\mu, x\rangle = \int_T x(t)\, d\mu(t) \tag{4}$$

and in particular for the Dirac measure δ_σ and the Lebesgue measure λ

$$\langle\delta_\sigma, x\rangle = x(\sigma) \tag{5}$$

$$\langle\lambda, x\rangle = \int_T x(t)\, dt \tag{6}$$

In this paper we shall restrict ourselves to two measures on the space ϕ_0: the Wiener–Feynman and the Uhlenbeck–Ornstein measures. The covariance $G(r, s)$ for the Wiener–Feynman measure is

$$\begin{aligned} G(r, s) = {} & Y^-(r - s)(r - t_a)(t_b - s)/(t_b - t_a) \\ & + Y^+(r - s)(s - t_a)(t_b - r)/(t_b - t_a) \end{aligned} \tag{7}$$

and that for Uhlenbeck–Ornstein measure is[4]

$$\begin{aligned} G(r, s) = {} & [2Y^-(r - s)\sinh(r - t_a)\sinh(t_b - s) \\ & + 2Y^+(r - s)\sinh(s - t_a)\sinh(t_b - r)]/\sinh(t_b - t_a) \end{aligned} \tag{8}$$

[3] The discussion of this section is entirely based on the results of Refs. 1 and 2. For the proof of the various propositions stated in this section the reader is referred to these papers.

[4] Y^+ and Y^- are the Heaviside step-up and step-down functions on T, respectively.

We shall need in the following a quadratic form on M defined as

$$W(\mu_i, \mu_j) = \int_T d\mu_i(r) \int_T d\mu_j(s)\, G(r, s) \tag{9}$$

We next state the following definition and propositions for the case of real Gaussian measures, which are similar to the corresponding results and propositions given in Refs. 1 and 2.

Definition. Let $\bar{\omega}$ be the measure on the vector space ϕ, which is the space of continuous functions x on the time interval $T = (t_a, t_b]$ such that the functions are fixed only at one end, say

$$x(t_a) = 0$$

ϕ_0 is a subspace of ϕ. We define a normalization constant N

$$1 = \int_{\phi_{xx}} d\omega_{xx}(x) = N^{-1} \int_{\phi_{xx}} d\bar{\omega}(x) \tag{10}$$

and the mean trajectory $\bar{x}(t)$

$$\bar{x}(t) \equiv \langle\langle \delta_t, x \rangle\rangle_{\phi_{xx}} = N^{-1} \int_{\phi_{xx}} x(t)\, d\bar{\omega}(x) \tag{11}$$

The integrals in Eqs. (10) and (11) can be performed using the mapping $P_n: \phi \to \mathbb{R}^n$ given by $x \to x_i = \langle \delta_{t_i}, x \rangle$, $t_a = t_0 \langle t_1 \langle t_2 \langle \cdots \langle t_n = t_b$. We have

$$\int_{\phi_{xx}} d\bar{\omega}(x) = \int_{\mathbb{R}^n} \delta(x_n - x) P(x_n | x_{n-1}) P(x_{n-1} | x_{n-2}) \times \cdots P(x_1 | x) \prod_{i=1}^{n} dx_i \tag{12}$$

For the Wiener–Feynman measure

$$P_{\text{WF}}(x_{k+1} | x_k) = \frac{1}{[2\pi(t_{k+1} - t_k)]^{1/2}} \exp - \frac{(x_{k+1} - x_k)^2}{2(t_{k+1} - t_k)} \tag{13}$$

and for the Uhlenbeck–Ornstein measure

$$P_{\text{UO}}(x_{k+1} | x_k) = \frac{1}{[2\pi\{1 - \exp[-2(t_{k+1} - t_k)]\}]^{1/2}} \times \exp - \frac{\{x_{k+1} - x_k \exp[-(t_{k+1} - t_k)]\}^2}{2\{1 - \exp[-2(t_{k+1} - t_k)]\}} \tag{14}$$

Proposition 1.

$$\langle\varphi_1(\langle\mu_1, x\rangle)\varphi_2(\langle\mu_2, x\rangle)\cdots\varphi_n(\langle\mu_n, x\rangle)\rangle_{\phi_0}$$
$$= \frac{1}{(2\pi)^{n/2}}\frac{1}{(\det W)^{1/2}}\int_{\mathbb{R}^n} du_1\cdots du_n\,\varphi_1(u_1)\cdots\varphi_n(u_n)$$
$$\times\exp\left(-\frac{1}{2}\sum_{i,j=1}^{n} u_i W_{ij}^{-1}u_j\right)$$
$$\langle\mu_i, x\rangle = u_i,\qquad i = 1,2,\cdots,n, \tag{15}$$

W is the matrix whose ij element is $W(\mu_i, \mu_j)$, which has been defined in Eq. (9).

Proposition 2. This is an obvious extension of Proposition 1:

$$\langle\varphi_1(\langle\mu_1, x-\bar{x}\rangle)\varphi_2(\langle\mu_2, x-\bar{x}\rangle)\cdots\varphi_n(\langle\mu_n, x-\bar{x}\rangle)\rangle_{\phi_{xx}}$$
$$= \langle\varphi_1(\langle\mu_1, x\rangle)\varphi_2(\langle\mu_2, x\rangle)\cdots\varphi_n(\langle\mu_n, x\rangle)\rangle_{\phi_0} \tag{16}$$

Proposition 3.

$$\int_{\mathbb{R}^n} F\left(\sum_{j=1}^{n} b_j x_j\right)\exp\left(-\sum_{j,k=1}^{n} x_j a_{jk} x_k\right)\prod_{i=1}^{n} dx_i$$
$$= \frac{\pi^{(n-1)/2}}{[c^2\det a]^{1/2}}\int_{\mathbb{R}} F(u)\exp\left(-\frac{u^2}{c^2}\right)du \tag{17}$$
$$c^2 = \sum_{i,j=1}^{n} b_i a_{ij}^{-1} b_j \tag{18}$$

The results given in this section are necessary and sufficient for the calculations of Sections 3 and 4.

3. PARTITION FUNCTION IN THE WIENER–FEYNMAN MEASURE

We consider a particle of mass unity in a potential $V(x)$. The partition function for this system is given by the following expression:

$$Z = \int_{\mathbb{R}} D\,dy\exp\left[-\int_0^\beta dt\,\langle\langle V(x(t))\rangle\rangle_y\right]$$
$$\times\left\langle\left\langle\exp\left[-\int_0^\beta dt\,\{V(x(t)) - \langle\langle V(x(t))\rangle\rangle_y\}\right]\right\rangle\right\rangle_y \tag{19}$$

$$\langle\langle\varphi(\langle\mu, x\rangle)\rangle\rangle_y = D^{-1}\int_{\mathbb{R}} dx\,N\left\langle\delta\left(\beta^{-1}\int_0^\beta x(t)\,dt - y\right)\varphi(\langle\mu, x\rangle)\right\rangle_{\phi_{xx}} \tag{20}$$

$$D = \int_{\mathbb{R}} dx\,N\left\langle\delta(\beta^{-1}\int_0^\beta x(t)\,dt - y)\right\rangle_{\phi_{xx}} \tag{21}$$
$$\beta = 1/kT$$

The exponential in the second term in the integrand of Eq. (19) can be expanded in a series and then one can take $\langle\langle\ \rangle\rangle_y$ of the terms of the expansion. The motivation to write the representation (19) for the partition function is the observation of Feynman[3] that one can save effort and increase accuracy in the calculation by expanding the potential in the integrand about the mean position given by

$$y = \beta^{-1} \int_0^\beta x(t)\, dt \tag{22}$$

It is therefore clear that we need moments of the type

$$\langle\langle V(x(\sigma)) \cdots V(x(M)) \cdots V(x(\rho))\rangle\rangle_y$$

We outline the method of calculation of such moments and in particular give in the following the details of the calculation of the moment of order two. We therefore calculate

$$\langle\langle \exp[-i\gamma x(\sigma) - i\zeta x(\rho)]\rangle\rangle_y \qquad \text{for} \quad \sigma \geqslant \rho$$

From Eq. (20) we have

$$\langle\langle \exp[-i\gamma x(\sigma) - i\zeta x(\rho)]\rangle\rangle_y$$
$$= D^{-1} \int_{-\infty}^{+\infty} dx\, N \left\langle \delta\left(\beta^{-1} \int_0^\beta x(t)\, dt - y\right) \exp[-i\gamma x(\sigma) - i\zeta x(\rho)] \right\rangle_{\phi_{xx}} \tag{23}$$

Using expressions (10), (11), and (13), we obtain

$$N = 1/(2\pi\beta)^{1/2}, \qquad \bar{x}(t) = x \tag{24}$$

We use the integral representation for the delta function

$$\delta\left(\frac{1}{\beta}\int_0^\beta x(t)\, dt - y\right) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{iky} \exp\left[-\frac{ik}{\beta}\int_0^\beta x(t)\, dt\right] dk \tag{25}$$

Using Proposition 2, we have

$$\left\langle \exp\left[-\frac{ik}{\beta}\int_0^\beta x(t)\, dt\right] \exp[-i\gamma x(\sigma)] \exp[-i\zeta x(\rho)] \right\rangle_{\phi_{xx}}$$
$$= \exp\left[-\frac{ik}{\beta}\int_0^\beta \bar{x}(t)\, dt\right] \exp[-i\gamma \bar{x}(\sigma)] \exp[-i\zeta \bar{x}(\rho)]$$
$$\times \langle \varphi_1(\langle \mu_1, x\rangle)\varphi_2(\langle \mu_2, x\rangle)\varphi_3(\langle \mu_3, x\rangle)\rangle_{\phi_0} \tag{26}$$

where $\mu_1 \to \lambda$, $\mu_2 \to \delta_\sigma$, $\mu_3 \to \delta_\rho$; $\langle \mu_1, x\rangle = u_1$, $\langle \mu_2, x\rangle = u_2$, $\langle \mu_3, x\rangle = u_3$; and

$$\begin{aligned} \varphi_1(\langle \mu_1, x\rangle) &= \exp[-(ik/\beta)u_1] \\ \varphi_2(\langle \mu_2, x\rangle) &= \exp(-i\gamma u_2) \\ \varphi_3(\langle \mu_3, x\rangle) &= \exp(-i\zeta u_3) \end{aligned} \tag{27}$$

We calculate the integral on the right-hand side of Eq. (26) using Propositions 1 and 3. The matrix W can be calculated using the expression for covariance given in Eq. (7) and taking $\mu_1 = \lambda$, $\mu_2 = \delta_\sigma$, and $\mu_3 = \delta_\rho$. The matrix W is found to be

$$W = \begin{pmatrix} \frac{1}{12}\beta^3 & \frac{1}{2}\sigma(\beta - \sigma) & \frac{1}{2}\rho(\beta - \rho) \\ \frac{1}{2}\sigma(\beta - \sigma) & (\sigma/\beta)(\beta - \sigma) & (\rho/\beta)(\beta - \sigma) \\ \frac{1}{2}\rho(\beta - \rho) & (\rho/\beta)(\beta - \sigma) & (\rho/\beta)(\beta - \rho) \end{pmatrix} \tag{28}$$

For this case F of Eq. (17) is exp and

$$b_1 = -ik/\beta, \qquad b_2 = -i\gamma, \qquad b_3 = -i\zeta \tag{29}$$

From Eqs. (18) and (28), we have

$$\begin{aligned} c^2 &= \sum_{i,j=1}^{3} b_i(2W_{ij})b_j \\ &= -2\left[\frac{k^2\beta}{12} + \frac{k\gamma\sigma(\beta - \rho)}{\beta} + \frac{\gamma^2\sigma(\beta - \sigma)}{\beta}\right. \\ &\quad \left. + \frac{k\zeta\rho(\beta - \rho)}{\beta} + \frac{2\gamma\zeta\rho(\beta - \sigma)}{\beta} + \frac{\zeta^2\rho(\beta - \rho)}{\beta}\right] \end{aligned} \tag{30}$$

We thus obtain

$$\begin{aligned} &\left\langle \exp\left[-\frac{ik}{\beta}\int_0^\beta x(t)\,dt\right] \exp[-i\gamma x(\sigma)] \exp[-i\zeta x(\rho)] \right\rangle_{\Phi_{xx}} \\ &= \exp[-ix(k + \gamma + \zeta)] \exp\frac{c^2}{4} \end{aligned} \tag{31}$$

A parallel calculation gives

$$D = N = 1/(2\pi\beta)^{1/2} \tag{32}$$

and

$$\begin{aligned} &\langle\langle \exp[-i\gamma x(\sigma) - i\zeta x(\rho)] \rangle\rangle_y \\ &\quad = \exp[-iy(\gamma + \zeta)] \exp\left(-\left\{\frac{\gamma^2\beta}{24} + \frac{\zeta^2\beta}{24}\right.\right. \\ &\quad\quad \left.\left. + \frac{\gamma\zeta}{2\beta}\left[\frac{\beta^2}{6} + (\sigma - \rho)^2 - \beta(\sigma - \rho)\right]\right\}\right)_{\sigma \geqslant \rho} \end{aligned} \tag{33}$$

Defining the Fourier transform of the potential

$$V(x(\sigma)) = \int_{-\infty}^{+\infty} d\gamma\, \{\exp[-i\gamma x(\sigma)]\} V(\gamma)$$

and using Eq. (33), we get

$$\int_0^\beta d\sigma \int_0^\beta d\rho \, \langle\langle V(x(\sigma)) V(x(\rho)) \rangle\rangle_y$$

$$= 2 \int_0^\beta d\sigma \int_0^\sigma d\rho \int_{-\infty}^{+\infty} d\gamma \int_{-\infty}^{+\infty} d\zeta \, V(\gamma) V(\zeta) \langle\langle \exp[-i\gamma x(\sigma) - i\zeta x(\rho)] \rangle\rangle_y \quad (34)$$

The moment $\langle\langle \exp[-i\gamma x(\sigma)] \rangle\rangle_y$ can be obtained by putting $\zeta = 0$ in Eq. (33). This gives

$$\langle\langle \exp[-i\gamma x(\sigma)] \rangle\rangle_y = \exp[-iy\gamma - (\gamma^2 \beta/24)] \quad (35)$$

Calculation of higher order moments presents no new difficulty.

4. PARTITION FUNCTION IN THE UHLENBECK–ORNSTEIN MEASURE

The Uhlenbeck–Ornstein function integral representation of the partition function arises from the Green's function of the dimensionless form of the Schrödinger–Bloch partial differential equation[5]

$$\frac{\partial \psi}{\partial t} = \left(\frac{\partial^2}{\partial x^2} - \frac{x^2}{4} - U(x) \right) \psi \quad (36)$$

where $U(x)$ is the nonquadratic part of the potential $V(x)$ in units of length and time,[(4,5)] which reduce the one-dimensional Schrödinger–Bloch equation to the form of Eq. (36). For a particle of mass unity, the end-point parameter β in the reduced units is

$$\beta = \frac{1}{kT} \left[\left(\frac{\partial^2 V}{\partial x^2} \right)_{x=0} \right]^{1/2} \quad (37)$$

The expression for the partition function in the Uhlenbeck–Ornstein measure is the same as that given through Eqs. (19)–(21) except for the difference that the right-hand side of Eq. (19) is to be multiplied by a factor of $\exp(-\beta/2)$ and $V(x)$ is to be replaced by $U(x)$. The integrals in the function space ϕ_0 and ϕ_{xx} are now performed with the real Gaussian measure of covariance $G(r, s)$ given in Eq. (8). Using expressions (10)–(12) and (14), a straightforward calculation gives

$$N = \frac{e^{\beta/2}}{[4\pi \sinh \beta]^{1/2}} \exp\left(-\frac{x^2}{2} \tanh \frac{\beta}{2} \right)$$

$$\bar{x}(t) = \frac{x \cosh(t - \frac{1}{2}\beta)}{\cosh(\beta/2)} \quad (38)$$

[5] For simplicity in notation we take $\hbar = 1$.

We next calculate $\langle\langle \exp[-i\gamma x(\sigma) \; -i\zeta x(\rho)\}\rangle\rangle_y$ for $\sigma \geqslant \rho$. We retain the notation of Section 3. The expressions for N and $\bar{x}(t)$ given in Eq. (38) are now to be used in Eq. (26). The matrix W for the covariance $G(r, s)$ given in Eq. (8) is found to be

$$W = \begin{pmatrix} 2\left(\beta - 2\tanh\frac{\beta}{2}\right) & \frac{4\sinh\frac{1}{2}(\beta-\sigma)}{\cosh\frac{1}{2}\beta}\sinh\frac{\sigma}{2} & \frac{4\sinh\frac{1}{2}(\beta-\rho)}{\cosh\frac{1}{2}\beta}\sinh\frac{\rho}{2} \\ \frac{4\sinh\frac{1}{2}(\beta-\sigma)}{\cosh\frac{1}{2}\beta}\sinh\frac{\sigma}{2} & \frac{2\sinh\sigma}{\sinh\beta}\sinh(\beta-\sigma) & \frac{2\sinh\rho}{\sinh\beta}\sinh(\beta-\sigma) \\ \frac{4\sinh\frac{1}{2}(\beta-\rho)}{\cosh\frac{1}{2}\beta}\sinh\frac{\rho}{2} & \frac{2\sinh\rho}{\sinh\beta}\sinh(\beta-\sigma) & \frac{2\sinh\rho}{\sinh\beta}\sinh(\beta-\rho) \end{pmatrix} \tag{39}$$

The expression for $c^2 = \sum_{i,j=1}^{3} b_i(2W_{ij})b_j$ is constructed from the matrix W given in Eq. (39). The result corresponding to the expression of Eq. (31) is

$$\left\langle \exp\left[-\frac{ik}{\beta}\int_0^\beta x(t)\,dt\right]\exp[-i\gamma x(\sigma)]\exp[-i\zeta x(\rho)]\right\rangle_{\Phi_{xx}}$$
$$= \exp\left\{-ix\left[\frac{2k}{\beta}\tanh\frac{\beta}{2} + \frac{\gamma\cosh(\sigma-\frac{1}{2}\beta)}{\cosh\frac{1}{2}\beta} + \frac{\zeta\cosh(\rho-\frac{1}{2}\beta)}{\cosh\frac{1}{2}\beta}\right]\right\}\exp\frac{c^2}{4} \tag{40}$$

From Eqs. (38) and (21), one easily finds that for this case

$$D = \frac{1}{4\sinh\frac{1}{2}\beta}\left(\frac{\beta}{\pi}\right)^{1/2} e^{\beta/2}\exp -\frac{\beta y^2}{4} \tag{41}$$

Substituting the expression of Eq. (40) into Eq. (23) and taking for D the right-hand side of Eq. (41), we get

$$\langle\langle \exp[-i\gamma x(\sigma) - i\zeta x(\rho)]\rangle\rangle_{y,(\sigma\geqslant\rho)}$$
$$= \exp\left[-\frac{1}{\beta}\left(\frac{\beta}{2}\coth\frac{\beta}{2} - 1\right)(\gamma^2+\zeta^2) + \frac{2\gamma\zeta}{\beta} - iy(\gamma+\zeta) - \gamma\zeta\left\{\coth\frac{\beta}{2}\cosh(\sigma-\rho) - \sinh(\sigma-\rho)\right\}\right] \tag{42}$$

and

$$\langle\langle \exp[-i\gamma x(\sigma)]\rangle\rangle_y = \exp\left[-\frac{1}{\beta}\left(\frac{\beta}{2}\coth\frac{\beta}{2} - 1\right)\gamma^2 - iy\gamma\right] \tag{43}$$

There is no loss of generality in having presented calculations of only second-order moments in this section and in Section 3. Extension of this program to higher order calculations is straightforward and can be performed on similar lines.

5. CONCLUSIONS

This paper is the first in a series which is based on the definition of function space integrals without a limiting procedure for expressions of the partition function in quantum statistical mechanics. The techniques would enable one to solve in a rigorous manner practical problems in statistical physics and especially enable the study of transport properties and correlation functions. One can choose at will measures on the topological vector space of functions which would give a better approximation to the study of thermodynamic properties in different temperature regions. This can be achieved by selecting appropriate covariances $G(r, s)$.

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