GIBBS EQUILIBRIUM AVERAGES AND BOGOLYUBOV MEASURE

D.P. Sankovich*

V. A. Steklov Mathematical Institute, Moscow, Russia

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Application of the functional integration methods in equilibrium statistical mechanics of quantum Bose-systems is considered. We show that Gibbs equilibrium averages of Bose-operators can be represented as path integrals over a special Gauss measure defined in the corresponding space of continuous functions. We consider some problems related to integration with respect to this measure.

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1. INTRODUCTION

Feynman [1] was the first to use functional integration in quantum physics. The construction of the Feynman functional (continual) integral shares common features with the Wiener integral. However, these integrals are essentially different [2].

The idea of expressing physical observables as continual integrals was developed in quantum field theory for representing Green functions. In due course, two such representation methods appeared almost simultaneously. One of them was based on formal integration of equations in variational derivatives for Green functions [3–5]. Bogolyubov [6] developed another approach proceeding from the representation of Green's functions in terms of vacuum expectations of chronological products, and the averaging operation over the boson vacuum was interpreted as a functional integral. The Bogolyubov functional integration method was used to study problems of gradient transformations for electrodynamic Green's functions and to investigate the Bloch–Nordsiek model. Bogolyubov returned to this construction within the framework of statistical mechanics when investigating the polaron model [7]. It was shown in [8] that the measure appearing in the Bogolyubov approach is the Gaussian measure in the related space of continuous functions. The Gibbs equilibrium means of chronological products of operators are expressed as functional integrals with respect to this measure.

2. BOGOLYUBOV'S MEASURE

If $\widehat{A}$ is a linear span of Bose operators and $\widehat{\Gamma}$ is a positive definite quadratic Hamiltonian, then the following formula holds [7]:

$$2\ln\langle e^{\widehat{A}}\rangle = \langle \widehat{A}^2\rangle. \tag{1}$$

Here $\langle\dots\rangle = \mathrm{Tr}\big[\dots e^{-\beta\widehat{\Gamma}}\big]/\mathrm{Tr}\, e^{-\beta\widehat{\Gamma}}$ denotes the Gibbs average with respect to the Hamiltonian $\widehat{\Gamma}$, β is the inverse temperature.

We consider the average

$$\left\langle T\exp\left[i\sum_{k=1}^{N+1}\nu_k\widehat{Q}(s_k)\right]\right\rangle, \tag{2}$$

where ν_k are real numbers and

$$0=s_1<s_2<\dots<s_k<\dots<s_N<s_{N+1}=\beta. \tag{3}$$

T is a chronological product. The operators $\widehat{Q}(s)$ and $\widehat{\Gamma}$ are given by

$$\widehat{Q}(s)=e^{s\widehat{\Gamma}}\hat{q}e^{-s\widehat{\Gamma}},\qquad \widehat{\Gamma}=\frac{\hat{p}^2}{2m}+\frac{m\omega^2}{2}\hat{q}^2,$$

which means that we consider the one-dimensional harmonic oscillator. $\hat{q}$ and $\hat{p}$ are the standard coordinate and momentum operators. Taking (1) into account, we can write

$$\left\langle T\exp\left[i\sum_{k=1}^{N+1}\nu_k\widehat{Q}(s_k)\right]\right\rangle = \exp\left\{-\frac{1}{2}\sum_{n=1}^{N+1}\sum_{m=1}^{N+1}\nu_n\nu_m\left\langle T\big[\widehat{Q}(s_n)\widehat{Q}(s_m)\big]\right\rangle\right\}.$$

We evaluate the average in the right-hand side of the last relation using the definition of chronological product, which leads to the formula

$$\left\langle T\big[\widehat{Q}(s_n)\widehat{Q}(s_m)\big]\right\rangle = \big(2m\omega(1-e^{-\beta\omega})\big)^{-1} \times\big(e^{-\omega|s_n-s_m|}+e^{-\beta\omega+\omega|s_n-s_m|}\big).$$

Thus, we have the following representation for the average (2):

$$\left\langle T\exp\left[i\sum_{k=1}^{N+1}\nu_k\widehat{Q}(s_k)\right]\right\rangle = e^{-\Omega(\{\nu_k\})} \tag{4}$$

*E-mail address: sankovch@mi.ras.ru

with the quadratic form in ν_k given by

$$\Omega(\{\nu_k\}) \equiv \frac{1}{2m\beta}\sum_{n=-\infty}^{\infty}\frac{\left|\sum_{k=1}^{N+1}\nu_k e^{2\pi i n s_k/\beta}\right|^2}{\omega^2+(2\pi n/\beta)^2}.$$

It is obvious, that $\Omega \geq 0$. Moreover, $\Omega = 0$ if and only if $\nu_1+\nu_{N+1}=0$ and $\nu_2=0,\ldots,\nu_N=0$.

Introducing new variables $\eta_1=\nu_1+\nu_{N+1}$, $\eta_2=\nu_2,\ldots,\eta_N=\nu_N$, we can rewrite (4) as

$$\left\langle T\exp\left[i\sum_{k=1}^{N+1}\nu_k\widehat{Q}(s_k)\right]\right\rangle = \exp\left(-\frac{1}{2}\sum_{j=1}^{N}\sum_{k=1}^{N}A_{jk}\eta_j\eta_k\right), \tag{5}$$

where

$$\sum_{j,k=1}^{N}A_{jk}\eta_j\eta_k = \frac{1}{m\beta}\sum_{n=-\infty}^{\infty}\frac{\left|\sum_{k=1}^{N}\eta_k e^{2\pi i n s_k/\beta}\right|^2}{\omega^2+(2\pi n/\beta)^2} \tag{6}$$

and the covariance matrix has the following elements:

$$A_{jk} = \frac{1}{2m\omega\sinh(\beta\omega/2)}\cosh\left(\frac{\beta\omega}{2}-\frac{\beta\omega}{N}|j-k|\right).$$

When deriving this formula, we defined partition (3) by the simple relation $s_j=\beta N^{-1}(j-1)$.

Consider the expression

$$\int\left\langle T\exp\left[i\sum_{k=1}^{N+1}\nu_k\widehat{Q}(s_k)\right]\right\rangle \times \exp\left\{-i\sum_{k=1}^{N+1}\nu_k q_k\right\}d\nu_1\ldots d\nu_N\,d\nu_{N+1},$$

where q_k are real numbers and the integration with respect to each variable ν_i goes over the entire real axis. Taking into account (5) and the known values of Gaussian integrals, we obtain

$$\begin{aligned}\frac{1}{(2\pi)^{N+1}}&\int\left\langle T\exp\left[i\sum_{k=1}^{N+1}\nu_k\widehat{Q}(s_k)\right]\right\rangle\\ \times\ &\exp\left\{-i\sum_{k=1}^{N+1}\nu_k q_k\right\}d\nu_1\ldots d\nu_N\,d\nu_{N+1}\\ =\ &\rho(q_1,q_2,\ldots,q_{N+1}),\end{aligned} \tag{7}$$

where

$$\rho(q_1,q_2,\ldots,q_{N+1}) = \frac{1}{\sqrt{(2\pi)^N}}\frac{\delta(q_1-q_{N+1})}{\sqrt{\det A}} \times\exp\left[-\frac{1}{2}\sum_{j,k=1}^{N}(A^{-1})_{jk}q_jq_k\right], \tag{8}$$

$\delta(q)$ is the Dirac delta function, and A^{-1} is the inverse covariance matrix inverse to A with the elements

$$\left(A^{-1}\right)_{ij} = \frac{m\omega}{\sinh(\frac{\beta\omega}{N})}\left(2\cosh\frac{\beta\omega}{N}\delta_{i,j}-\delta_{i,j+1}-\delta_{i,j-1}\right).$$

It follows from (8) that

$$\rho\geq 0,\qquad \int\rho\,dq_1\ldots dq_{N+1}=1. \tag{9}$$

Using relation (7), we can evaluate averages of the form

$$\left\langle T\left[f(\widehat{Q}(s_1),\ldots,\widehat{Q}(s_{N+1}))\right]\right\rangle.$$

Indeed, we recall the complex Fourier formula

$$f(Q_1,\ldots,Q_{N+1}) = \frac{1}{(2\pi)^{N+1}}\int f(q_1,\ldots,q_{N+1}) \times\exp\left\{i\sum_{j=1}^{N}\nu_j(Q_j-q_j)\right\}dq_1\ldots dq_{N+1}\,d\nu_1\ldots d\nu_{N+1}.$$

Since the operators $\widehat{Q}(s_j)$ commute under sign of the T-product, we have

$$\begin{aligned}&\left\langle T\left[f\left(\widehat{Q}(s_1),\ldots,\widehat{Q}(s_{N+1})\right)\right]\right\rangle\\ &=\int f(q_1,\ldots,q_{N+1})\\ &\times\ \rho(q_1,\ldots,q_{N+1})\,dq_1\ldots dq_{N+1}.\end{aligned} \tag{10}$$

Taking into account properties (9), we see that

$$\begin{aligned}&0\leq\left\langle T\left[f\left(\widehat{Q}(s_1),\ldots,\widehat{Q}(s_{N+1})\right)\right]\right\rangle\leq M,\\ &\text{if}\quad 0\leq f\left(\widehat{Q}(s_1),\ldots,\widehat{Q}(s_{N+1})\right)\leq M.\end{aligned} \tag{11}$$

Now, consider the functionals $F(q)$ on the real functions ("trajectories") $q(s)$ defined on the segment $0\leq s\leq\beta$. Let us construct the integral

$$I\equiv\int F(q)\,d\mu \tag{12}$$

with respect to the corresponding measure.

We first consider the subset of "special functionals" [7] that are continuous functions of a finite number N of variables, $F^{(N)}(q)\equiv\Phi(q_1,q_2,\ldots,q_N)$, where $q_j=q(s_j)$. In this case, we obtain

$$\begin{aligned}I^{(N)} &= \int\Phi(q_1,q_2,\ldots,q_N)\\ &\times\ \rho(q_1,q_2,\ldots,q_N)\,dq_1\,dq_2\ldots dq_N.\end{aligned} \tag{13}$$

Then, formulas (10) and (11) imply that

$$\left\langle T\left[F^{(N)}(\widehat{Q})\right]\right\rangle = \int F^{(N)}(q)\,d\mu$$

and that $\left\langle T\left[F^{(N)}(\widehat{Q})\right]\right\rangle\geq 0$ if $F^{(N)}(q)\geq 0$ for arbitrary real numbers $q_1,q_2,\ldots,q_N$. We now consider a sequence of functions $\{q_N(s)\}$, $N=1,2,\ldots$, that are defined as follows:

$$\begin{aligned}&q_N(s)=q(s_j), s_j\leq s<s_{j+1}, j=1,2,\ldots,N,\\ &q_N(\beta)=q(\beta).\end{aligned} \tag{14}$$

The set of points $\{s_j\}$ is the partition (3) of the segment $[0,\beta]$. We suppose that $|s_{j+1}-s_j|\leq\Delta s$ for $j=1,2,\ldots,N$ and assume that $\Delta s\to 0$ as $N\to\infty$. Then the sequence of step functions (14) uniformly tends to the function $q(s)$. Path integral (12) can be defined as the limit $N\to\infty$ of integrals (13), defined on the subset of special functionals, because the functionals $F(q_N(s))$ belong to this subset $I = \lim_{N\to\infty} I^{(N)}$.

Consider the space $C^\circ[0,\beta]$ of continuous functions $q(s)$ defined on the segment $[0,\beta]$ that satisfy the condition $q(0) = q(\beta)$. This is a metric space with respect to the uniform metric $\rho(q,p) = \sup_{s\in[0,\beta]} |q(s) - p(s)|$. The square matrix $A = (A_{jk})$ of order N is positive and symmetrical, i.e., the mapping $(j,k) \to A_{jk}$ is a positive-type kernel on the set $\{1,2,\dots,N\}$. Hence, we can speak of the Gaussian measure γ_A on the space R^N with the covariance A. By the Stone–Weierstrass theorem, the corresponding set of special functional is dense in the set of all continuous functions defined on the space $C^\circ[0,\beta]$. In the space $C^\circ[0,\beta]$, we can introduce a σ-algebra generated by quasi intervals (cylindrical sets). This σ-algebra coincides with the σ-algebra generated by the sets that are open in the metric ρ. Extending the Gaussian measure from the quasi intervals to their Borel closure, we obtain a Gaussian measure in the space $C^\circ[0,\beta]$.

3. GIBBS EQUILIBRIUM AVERAGES

So we see that the Gaussian measure μ_{B} with zero average and the correlation function

$$B(t,s) = \frac{1}{2m\omega\sinh(\beta\omega/2)}\cosh\left(\omega|t-s| - \frac{\beta\omega}{2}\right) \tag{15}$$

is defined in the space $X = C^\circ[0,\beta]$ of continuous functions on the interval $[0,\beta]$ with the uniform metric $\rho = \max_{t\in[0,\beta]}\big|x(t) - y(t)\big|$ that satisfy the condition $x(0) = x(\beta)$. Measurable functionals $F(x)$ are considered on the space with measure $\{X, G, \mu_{\mathrm{B}}\}$, where G is an isolated σ algebra of subsets in this space. In this case, the formula

$$\big\langle T\big[F\big(\widehat{Q}(t)\big)\big]\big\rangle_{\widehat{\Gamma}} = \int_X F\big(x(t)\big)\,d\mu_{\mathrm{B}}(x) \tag{16}$$

holds for the Gibbs equilibrium mean of the T-product taken with respect to the Hamiltonian $\widehat{\Gamma}$ of the harmonic oscillator; the integral is understood as the Daniell integral over the space X,

$$\widehat{\Gamma} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{q}^2,\ \ \widehat{Q}(t) = e^{t\widehat{\Gamma}}\hat{q}e^{-t\widehat{\Gamma}},$$

$$\langle\,\cdot\,\rangle_{\widehat{\Gamma}} = \frac{\mathrm{Tr}(\,\cdot\, e^{-\beta\widehat{\Gamma}})}{\mathrm{Tr}\,e^{-\beta\widehat{\Gamma}}},$$

where $\hat{q}$ and $\hat{p}$ are the respective coordinate and momentum operators of a particle with mass m that satisfy the commutation relation $[\hat{q},\hat{p}] = i$ ($\hbar = 1$ is assumed), β is the reciprocal of the temperature, and ω is the eigenfrequency of the oscillator ($\beta > 0$, $\omega > 0$.) The average in formula (16) exists and is finite for an integrable functional $F(x)$. The measure μ_{B} thus defined is called the Bogolyubov measure.

Note also that in the case of the Bogolyubov measure, the function $G(t,s) = -mB(t,s)$ is the Green's function of the boundary value problem:

$$\begin{cases} y'' - \omega^2 y = 0, \\ y(0) = y(\beta), \\ y'(0) = y'(\beta) \end{cases}$$

on the segment $[0,\beta]$.

Let $a_1, a_2, \dots, a_n$ be linearly independent elements in a separable Hilbert space H whose closure is the support of a measure μ and which is dense almost everywhere in X. Then,

$$\int_X F\big[(a_1,x),(a_2,x),\dots,(a_n,x)\big]\,d\mu(x) = (2\pi)^{-n/2}\frac{1}{\sqrt{\det A}}\int_{R^n} e^{-(A^{-1}u,u)/2}F(u)\,du \tag{17}$$

if one of the integrals in (17) exists, where A is the matrix of the elements $a_{ij} = (a_i,a_j)_H$, $i,j = 1,2,\dots,n$, $u = (u_1,u_2,\dots,u_n)$, and $du = du_1 du_2\cdots du_n$.

For example, in the case of the Bogolyubov measure:

$$\langle\hat{q}^2\rangle_{\widehat{\Gamma}} = \int_X x^2(t)\,d\mu_{\mathrm{B}}(x) = B(t,t) = \frac{1}{2m\omega}\coth\frac{\beta\omega}{2},$$

$$\langle e^{a\hat{q}^2}\rangle_{\widehat{\Gamma}} = \sum_{n=0}^{\infty}\frac{(2n)!}{2^n(n!)^2}\big(a\langle\hat{q}^2\rangle_{\widehat{\Gamma}}\big)^n = \frac{1}{\sqrt{1 - a\coth(\beta\omega/2)/(m\omega)}}, \tag{18}$$

where we should assume that $-m\omega\tanh(\beta\omega/2) \le a < m\omega\tanh(\beta\omega/2)$ in the second formula.

Consider the family of operators $\{T(\beta) : 0 \le \beta < \infty\}$ that act in the space $L^2(R)$ by the rule

$$(T(\beta)f)(x) = \int_X d\mu_{\mathrm{B}}(y)\,f\bigg(\int_0^\beta y(t)\,dt + x\bigg). \tag{19}$$

It is obvious that $T(0) = I$. We obtain

$$(T(\beta)f)(x) = \sqrt{\frac{m\omega^2}{2\pi\beta}}\int_{-\infty}^{\infty} f(y)\exp\left[-\frac{(y-x)^2 m\omega^2}{2\beta}\right]dy. \tag{20}$$

Formula (20) is the well-known formula for the free semigroup in the case of the heat equation. Thus, the family of operators (19) is indeed a strongly continuous semigroup in the space $L^2(R)$. The generator of the semigroup is given by

$$L = \frac{1}{2m\omega^2}\frac{d^2}{dx^2},$$

and for any function $f \in L^2(R)$, the function $u(\beta,x) = (T(\beta)f)(x)$ is the solution of the Bloch equation

$$\frac{\partial u}{\partial\beta} = \frac{1}{2m\omega^2}\frac{\partial^2 u}{\partial x^2}$$

subject to the initial condition $u(0,x) = f(x)$. Formula (19) implies the relation between the Bogolyubov and Wiener measures

$$\int_{C^\circ[0,m\omega^2 t]} f\left(x + \int_0^{m\omega^2 t} y(\tau)\,d\tau\right) d\mu_{\mathrm{B}}(y)$$
$$= \int_{C_0^t} f(y(t)+x)\,d\mu_{\mathrm{W}}(y),$$

where C_0^t is the space of continuous functions on $[0,t]$ that vanish at zero.

A Gaussian random process with a Bogolyubov measure has independent increments, i.e., the random variables $y(t_2)-y(t_1),\dots,y(t_n)-y(t_{n-1})$, where

$$y(t) = \omega^{-1}x(t) + \int_0^t x(\tau)\,d\tau, \quad 0 \le t \le \beta, \tag{21}$$

are independent for any $0 < t_1 < t_2 < \cdots < t_n \le \beta$.

4. THE INEQUALITY

Consider a system with a Hamiltonian $\widehat{H} = \widehat{\Gamma} + \widehat{V}$, where $\widehat{V} = V(\hat{q})$ is the interaction, and consider a one-parameter family of Hamiltonians, $\widehat{H}(h) = \widehat{\Gamma}(h) + \widehat{V}, \quad h \in R,$

$$\widehat{\Gamma}(h) = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}(\hat{q}-h)^2.$$

The partition function $Z(h) = \operatorname{Tr} e^{-\beta\widehat{H}(h)}$ of the system under consideration becomes $Z(h) = \operatorname{Tr} e^{-\beta[\widehat{\Gamma}+V(\hat{q}+h)]}$ after the canonical transformation $\hat{q} - h \to \hat{q}$. We will assume that the interaction potential is nonnegative and symmetric, i.e., $V(x) \ge 0, \quad V(x) = V(-x)$. Using the operator of chronological ordering, we can write [7]

$$e^{-\beta(\widehat{\Gamma}+\widehat{V})} = e^{-\beta\widehat{\Gamma}} T \exp\left(-\int_0^\beta ds\, e^{s\widehat{\Gamma}}\widehat{V}e^{-s\widehat{\Gamma}}\right).$$

Then,

$$R(h) \equiv \frac{\operatorname{Tr} e^{-\beta\widehat{H}(h)}}{\operatorname{Tr} e^{-\beta\widehat{\Gamma}}}$$
$$= \left\langle T\exp\left[-\textstyle\int_0^\beta ds\, V\big(\widehat{Q}(s)+h\big)\right]\right\rangle_{\widehat{\Gamma}}. \tag{22}$$

Expressing (22) in terms of the Bogolyubov functional integral, we obtain

$$R(h) = \int_X \exp\left[-\int_0^\beta ds\, V\big(x(s)+h\big)\right] d\mu_{\mathrm{B}}(x).$$

We can prove that

$$R(h) \le R(0). \tag{23}$$

Condition (23) implies, in particular, that

$$(\hat{q},\hat{q})_{\widehat{H}} \le \frac{1}{\beta m\omega^2}, \tag{24}$$

where the Bogolyubov inner product of arbitrary operators $\widehat{A}$ and $\widehat{B}$ is defined as

$$(\widehat{A},\widehat{B})_{\widehat{H}} = \frac{1}{\beta \operatorname{Tr} e^{-\beta\widehat{H}}} \int_0^\beta ds\, \operatorname{Tr}\big[e^{-s\widehat{H}}\widehat{A}e^{-(\beta-s)\widehat{H}}\widehat{B}\big].$$

If we pass from the operators $\hat{q}$ and $\hat{p}$ to operators $\hat{b}$ and $\hat{b}^\dagger$ by the relations

$$\hat{q} = \frac{1}{\sqrt{2m\omega}}(\hat{b}+\hat{b}^\dagger), \qquad \hat{p} = i\sqrt{\frac{m\omega}{2}}\,(\hat{b}^\dagger - \hat{b})$$

and take into account the selection rules for equilibrium averages with respect to a quadratic Hamiltonian, we can rewrite inequality (24) as $\big(\hat{b}^\dagger,\hat{b}\big)_{\widehat{H}} \le (\beta\omega)^{-1}$.

Relation (24) can be used to derive an inequality for the Gibbs equilibrium average $\langle\hat{q}^2\rangle_{\widehat{H}}$. To this end, the Falk–Bruch inequality [9] should be used. Let

$$g = \langle\hat{q}^2\rangle_{\widehat{H}}, \;\; b = (\hat{q},\hat{q})_{\widehat{H}}, \;\; c = \big\langle\big[\hat{q},[\beta\widehat{H},\hat{q}]\big]\big\rangle_{\widehat{H}}.$$

Suppose that the upper estimates $b \le b_0$ and $c \le c_0$ hold. Then,

$$g \le g_0 \equiv \frac{1}{2}\sqrt{c_0 b_0}\,\coth\sqrt{\frac{c_0}{4b_0}}.$$

In our case $b_0 = (\beta m\omega^2)^{-1}$, $c_0 = \beta/m$, and the above inequality yields

$$\langle\hat{q}^2\rangle_{\widehat{H}} \le \frac{1}{2m\omega}\coth\frac{\beta\omega}{2} = \langle\hat{q}^2\rangle_{\widehat{\Gamma}}.$$

Condition (23) is an example of the so-called Gaussian domination condition [10], and condition (24) which follows from (23), is an example of the so-called local Gaussian domination condition [11], which plays an important role in phase transition theory.

5. CONCLUSIONS

A review of some recent developments in the theory of integration with respect to the Bogolyubov measure that arises in the statistical equilibrium theory for quantum systems is presented. It is shown that the Gibbs equilibrium averages of Bose operators can be represented as functional integrals with respect to this measure. The metric and dynamic properties of Bogolyubov trajectories in the corresponding functional space are established. Certain functional integrals with respect to the Bogolyubov measure are calculated. A certain useful inequality for traces is proved. For a detailed review of the theory of Bogolyubov functional integral, with extensive references in the literature, see Ref. [12].

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ГИББСОВСКИЕ РАВНОВЕСНЫЕ СРЕДНИЕ И МЕРА БОГОЛЮБОВА

Д.П. Санкович

Рассмотрено применение методов функционального интегрирования в квантовой равновесной статистической механике бозе-систем. Показано, что гиббсовские равновесные средние бозе-операторов могут быть представлены в виде функциональных интегралов по специальной гауссовой мере, определенной в соответствующем пространстве непрерывных функций. Рассмотрены некоторые вопросы, относящиеся к интегрированию по данной мере.

ГИБСОВСЬКІ РІВНОВАЖНІ СЕРЕДНІ І МІРА БОГОЛЮБОВА

Д.П. Санкович

Розглянуто застосування методів функціонального інтегрування у квантовій рівноважній статистичній механіці бозе-систем. Показано, що гибсовські рівноважні середні операторів можуть бути представлені у вигляді функціональних інтегралів по спеціальній гаусовій мірі, визначеній у відповідному просторі безперервних функцій. Розглянуті деякі питання, що відносяться до інтегрування по даній мірі.