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NOTE ON PATH INTEGRAL QUANTIZATION
OF HYDROGEN ATOM

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Abstract

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For path integrals, whose integration measures are generated by stochastic processes of a definite form (Stratonovich-type equations are a local form for stochastic differential equations of these processes) it has been shown that under quantization of hydrogen atom the reparametrization and reduction Jacobians are mutually cancelled.

Аннотация

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Для континуальных интегралов, чьи меры интегрирования порождены случайными процессами определенного вида (локальной формой для стохастических дифференциальных уравнений этих процессов являются уравнения типа Стратоновича) показано, что при квантовании атома водорода происходит взаимное сокращение якобианов репараметризации и редукции.

1. The path integral quantization procedure for hydrogen atom was proposed in ref./1/. This procedure involves two transformations of the path integral. The first one is connected with Kustaanheimo - Stiefel transformation /2/, and the second one is the path reparametrization transformation (it is also called a change of the time variable). The forthcoming papers, where the Jacobians of these two transformations had been calculated in a "discrete approach to the path integral", were criticized by Kleinert in ref./3/

In the present paper hydrogen atom is quantized in the approach based on "the continuum version of path integrals". By this we imply the integrals over measure, generated by stochastic processes. For our path integrals the stochastic processes will be given as solutions of stochastic differential equations on manifolds, (Stratonovich-type equations being a local form of these equations). In a flat case the integrals determined according to the symmetric ordering rule will be used as discrete approximations of our path integrals. Discrete approximations for the manifold were considered in ref./4/.

In the present paper we show how the path integration method developed on the basis of the stochastic processes in refs./5,6/, may be applied to a particular case of hydrogen atom quantization. Earlier the methods of the stochastic process theory for hydrogen atom quantization were used in refs./5,7/.

2. Two independent transformations should be realized in the path integral, i.e., path reparametrization and Kustaanheimo-Stiefel transformation.

The path integral symbol

$$K(x_b, t_b; x_a, t_a) = \int_{\substack{x(t_a)=x_a \\ x(t_b)=x_b}} \frac{Dx^3 Dp^3}{[2\pi\hbar]^3} \exp\left(\frac{i}{\hbar} \int_{t_a}^{t_b} dt \left(\tilde{p}\dot{x} - \frac{\tilde{p}^2}{2m} + \frac{e^2}{r}\right)\right) \quad (1)$$

gives a representation for the Green's functions of hydrogen atom. By this symbol we understand an integral over the measure, generated by a corresponding stochastic process. Consequently, the calculations in this paper will, in fact, be carried out for the Wiener integrals rather than for the Feynman path integrals.

Besides instead of the path integral symbols over configuration space, which are usually related to the Wiener integrals, we shall use the path integral symbols over the phase space.

The formula for the transformation of the path integral symbol as a result of path reparametrization was earlier derived in refs. /6/. According to this formula the Green's functions for two quantum-mechanical problems, if the paths are reparametrized in a new time $s(t)=$

$= \int_{t_a}^t \exp(2\phi(x(\tau))) d\tau$, are connected in the following way

$$\begin{aligned} & g^{-1/4}(x_a) g^{-1/4}(x_b) \int_{\substack{x(t_a)=x_a \\ x(t_b)=x_b}} \prod_{\alpha=1}^n \frac{Dx^\alpha(t) Dp_\alpha(t)}{[2\pi\hbar]^n} \exp\left(\frac{i}{\hbar} \int_{t_a}^{t_b} (p_\alpha \dot{x}^\alpha - \right. \\ & \left. - \frac{1}{2m} g^{\alpha\beta} p_\alpha p_\beta - V) dt\right) = \exp\left(\frac{n-2}{2} \phi(x_a)\right) \cdot \\ & \cdot \exp\left(\frac{n-2}{2} \phi(x_b)\right) \int \frac{dE}{2\pi\hbar} \exp\left(-\frac{i}{\hbar} E(t_b - t_a)\right) \int_{s_a}^{s_b} ds_b \cdot \\ & \cdot g^{-1/4}(x_a) g^{-1/4}(x_b) \int_{\substack{x(s_a)=x_a \\ x(s_b)=x_b}} \prod_{\alpha=1}^n \frac{Dx^\alpha(s) Dp_\alpha(s)}{(2\pi\hbar)^n} \exp\left(\frac{i}{\hbar} \int_{s_a}^{s_b} \left(p_\alpha \frac{dx^\alpha}{ds} - \right. \right. \\ & \left. \left. - \frac{1}{2m} g^{\alpha\beta} p_\alpha p_\beta - \frac{\hbar^2}{2m} \left(\frac{n-2}{4(n-1)}\right) (\tilde{R} e^{-2\phi} R) + E e^{-2\phi} - e^{-2\phi} V\right) ds\right), \quad (2) \end{aligned}$$

where $\tilde{g}_{\alpha\beta} = e^{2\phi} g_{\alpha\beta}$, \tilde{R} and R are scalar curvatures of manifolds with metrics $\tilde{g}_{\alpha\beta}$ and $g_{\alpha\beta}$, $\tilde{R} = e^{-2\phi} (R - 2(n-1)\Delta_1\phi - (n-1)(n-2)\Delta_1^2\phi)$, (here

$$\Delta_1\phi = g^{\alpha\beta} \frac{\partial\phi}{\partial x^\alpha} \frac{\partial\phi}{\partial x^\beta}, \quad \Delta_2\phi = g^{-1/2} \partial_\alpha g^{1/2} g^{\alpha\beta} \partial_\beta \phi, \quad g = \det g_{\alpha\beta}.$$

The infinitesimal generator of the evolution operator, whose kernel is presented with the path integral symbol from the R.H.S. of (2), is Laplace-Beltrami operator on the manifold with metric $g_{\alpha\beta}$. The same quantization rule is used for the Hamiltonian from the RHS of formula (2). Applying (2) to our case, when $dt/ds = r (r = \sqrt{x_1^2 + x_2^2 + x_3^2})$ we obtain

$$\begin{aligned} K(x_b, t_b; x_a, t_a) &= r_a^{-1/4} r_b^{-1/4} \int \frac{dE}{2\pi\hbar} \exp\left(-\frac{i}{\hbar} E(t_b - t_a)\right) \times \\ &\times \int_{s_a}^{\infty} ds_b \exp\left(\frac{i}{\hbar} e^2 (s_b - s_a)\right) r_a^{3/4} r_b^{3/4} \int_{\substack{x(s_a) = x_a \\ x(s_b) = x_b}} \frac{D^3 x D^3 p}{[2\pi\hbar]^3} \times \\ &\times \exp\left(\frac{i}{\hbar} \int_{s_a}^{s_b} \left(p_i \frac{dx^i}{ds} - \frac{r\vec{p}^2}{2m} + Er - \left(\frac{\hbar^2}{2m}\right) \frac{3}{16r}\right) ds\right), \end{aligned} \quad (3)$$

where the factor $\exp(i/\hbar e^2 (s_b - s_a))$, which results from reparametrization is taken out of the path integral. From (3) it is seen that the reparametrization Jacobian for our path integral is different from identity.

3. It is convenient to consider Kustaanheimo-Stiefel transformation in the path integral in spherical coordinates. The transformation to the spherical coordinates is a homogeneous point transformation. To realize such transformation in the path integral we shall apply to an analogous transformation in stochastic processes.

In stochastic processes a phase transformation of processes is an analogue for the homogeneous point transformation. For it one knows the relation between the densities before and after transformation /8/. Since each density admits representation in the form of an integral over the measure, generated by stochastic process, then the relation between the probability densities is, in fact, the one between such integrals. But in the path integration it is also demanded that the measures should be generated by the pro-

cesses of a similar type. In our case the processes should be described with such stochastic differential equations on manifolds, whose local, (i.e., on separate charts) stochastic differential equations are the ones of the Stratonovich type. The differential generators for such processes are Laplace-Beltrami operators. After additional transformation of the obtained relation to the required form, one can represent it as a relation between the density probabilities in the form of a rule for the transformation of the path integral symbol.

According to this rule the symbolic measure for the path integral under homogeneous point transformations $x^i = f^i(y), p_j = p_i(\partial f^i / \partial y^j)$ is not invariant

$$\prod_{i=1}^n \frac{Dx^i(t) Dp_i(t)}{[2\pi\hbar]^n} = \left| \frac{\partial(x^1, \dots, x^n)}{\partial(y^1, \dots, y^n)} \right|_{t_a}^{1/2} \times$$

$$\times \left| \frac{\partial(x^1, \dots, x^n)}{\partial(y^1, \dots, y^n)} \right|_{t_b}^{1/2} \prod_{i=1}^n \frac{Dy^i(t) Dp_i(t)}{[2\pi\hbar]^n}$$

and in the remaining terms of the path integral, including boundary delta-function and factors $g^{1/4}(x_a)g^{-1/4}(x_b)$ as well, we make a standard substitution. In this, for classical Hamiltonians before and after transformation the quantization rule is still true: for the classical Hamiltonian

$$H = \frac{1}{2m} g^{\alpha\beta}(x) p_\alpha p_\beta + a^\alpha(x) p_\alpha$$

the Hamiltonian operator will be

$$H = -\frac{\hbar^2}{2m} \Delta + (-i\hbar) \left[a^\alpha \frac{\partial}{\partial x^\alpha} + \frac{1}{2} g^{-1/2} \frac{\partial(g^{1/2} a^\alpha)}{\partial x^\alpha} \right], \quad (4)$$

where $\Delta = g^{-1/2} \partial_\alpha g^{\alpha\beta} g^{1/2} \partial_\beta$ is Laplace-Beltrami operator.

The wave functions have been normalized in the following way

$$(\psi, \psi) = \int |\psi|^2 \sqrt{g} dx^1 \dots dx^n.$$

Note, that only insignificant modifications of our earlier reasoning are re-quired for application of such a quantization rule to the Hamiltonians including the terms linear in moments. Under path integral transformation the

term without the derivative from (4) must be treated as a potential term. Then its changes after homogeneous point transformation may be taken into account, assuming that a usual substitution is made in the path integral symbol and quantization rule (4) holds.

It should also be noted that similar to one-dimensional case in /9/ it is simple to follow the derivation of the relation between the probability densities using the differential equations for these densities.

After transition to spherical coordinates in (3)

$$x^1 = r \sin \theta \cos \varphi, \quad x^2 = r \sin \theta \sin \varphi, \quad x^3 = r \cos \theta \quad (5)$$

we obtain ($' = d/ds$)

$$K = r_a^{-1/4} r_b^{-1/4} \int \frac{dE}{2\pi\hbar} \exp\left(-\frac{i}{\hbar} E(t_b - t_a)\right) \int_{s_a}^{s_b} ds_b \exp\left(\frac{i}{\hbar} e^2 (s_b - s_a)\right) \times$$

$$\times (r_a \sin^2 \theta_a)^{-1/4} (r_b \sin^2 \theta_b)^{-1/4} \times$$

$$\int \frac{D(r, \theta, \varphi) D(p_r, p_\theta, p_\varphi)}{[2\pi\hbar]^3} \times$$

$$\begin{matrix} (r, \theta, \varphi)(s_a) = (r_a, \theta_a, \varphi_a) \\ (r, \theta, \varphi)(s_b) = (r_b, \theta_b, \varphi_b) \end{matrix}$$

$$\times \exp\left(\frac{i}{\hbar} \int_{s_a}^{s_b} [p_r r' + p_\theta \theta' + p_\varphi \varphi' - \frac{1}{2m}(r p_r^2 + \frac{1}{r} p_\theta^2 + \frac{1}{r \sin^2 \theta} p_\varphi^2) + \right.$$

$$\left. + E r - \left(\frac{\hbar^2}{2m}\right) \frac{3}{16r} \right] ds), \quad (6)$$

where the boundary conditions are already the usual delta functions over r , θ and φ .

4. The Kustaaheimo-Stiefel transformation which expresses the variables

$$\begin{aligned} u_1 &= \sqrt{r} \sin \frac{\theta}{2} \cos \left[\frac{1}{2}(\alpha + \varphi) \right], & u_2 &= \sqrt{r} \cos \frac{\theta}{2} \sin \left[\frac{1}{2}(\alpha - \varphi) \right] \\ u_3 &= \sqrt{r} \cos \frac{\theta}{2} \cos \left[\frac{1}{2}(\alpha - \varphi) \right], & u_4 &= \sqrt{r} \sin \frac{\theta}{2} \sin \left[\frac{1}{2}(\alpha + \varphi) \right] \end{aligned} \quad (7)$$

(α varies from 0 upto 4π) through the variables (x^1, x^2, x^3) from (5), is connected with the problem of reduction of a dynamical system with symmetry /10,11/. In the hydrogen atom problem on $T^*\dot{R}^4$ ($\dot{R}^4 = R^4 - \{0\}$) there has been defined a dynamical system with $U(1) = S^1$ symmetry. The zero-moment reduction for this system proceeds in such a way that the reduced phase space is diffeomorphic to $T^*\dot{R}^3$ /11/ and Kustaanheimo-Stiefel transformation extends the Hopf mapping to $\pi: \dot{R}^4 \rightarrow \dot{R}^3$.

We shall now go over to the path integral reduction. But first we shall see how this reduction is realized in the equations for the Green's functions. The relation for the Green's function derived from these considerations, will be re-written as a relation between path integral symbols.

Let us make use of Manoukian's paper /12/, correcting uncertainties in the paper. From this paper it follows that the functions G_0 and G , satisfying the equations

$$[i\hbar \frac{\partial}{\partial s} + \frac{\hbar^2}{2m} (r \frac{\partial^2}{\partial r^2} + 2 \frac{\partial}{\partial r} + \frac{1}{r} \frac{\partial^2}{\partial \theta^2} + \frac{1}{r} \operatorname{ctg} \theta \frac{\partial}{\partial \theta} + \frac{1}{r \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}) - V(r)]_b G_0 = i\hbar \delta(s_b - s_a) r_b^{-1} \sin^{-1} \theta_b \delta(r_b - r_a) \delta(\theta_b - \theta_a) \delta(\varphi_b - \varphi_a), \quad (8)$$

and

$$[i\hbar \frac{\partial}{\partial s} + \frac{\hbar^2}{2m} (r \frac{\partial^2}{\partial r^2} + 2 \frac{\partial}{\partial r} + \frac{1}{r} \frac{\partial^2}{\partial \theta^2} + \frac{1}{r} \operatorname{ctg} \theta \frac{\partial}{\partial \theta} + \frac{1}{r \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} + \frac{1}{r \sin^2 \theta} \frac{\partial^2}{\partial \alpha^2} + \frac{2 \cos \theta}{r \sin^2 \theta} \frac{\partial^2}{\partial \varphi \partial \alpha}) - V(r)]_b G = i\hbar \delta(s_b - s_a) (16r_b^{-1}) \sin^{-1} \theta_b \delta(r_b - r_a) \delta(\theta_b - \theta_a) \delta(\varphi_b - \varphi_a) \delta(\alpha_b - \alpha_a) \quad (9)$$

([.]_b imply that the operator acts on the variables with index b), are connected through the relation

$$G_0 = \frac{1}{16} \int_0^{4\pi} d\alpha_b G. \quad (10)$$

In its turn G can be presented in the form

$$G = \frac{4}{\pi} \sum_{M=-\infty}^{\infty} \exp(-\frac{iM}{2} (\alpha_b - \alpha_a)) G_M,$$

where G_M is an α -independent function.

The zero-momentum reduction means here, that out of all G_M we choose the function with a zero value of M .

From (8) it is seen that G_0 acts in the Hilbert space with a scalar product $(\Psi\Psi) = \int |\Psi|^2 r \sin\theta dr d\theta d\varphi$. However the path integral in the R.H.S. of (6) provides a representation for the Green's function, defined in the Hilbert space with a scalar product $(\Psi\Psi) = \int |\Psi|^2 r^{1/2} \sin\theta dr d\theta d\varphi$. Isometric transformation of one Hilbert space into another establishes the following relations between the Green's functions from these spaces and between differential generators of the evolution operators.

$$\tilde{G} = r_b^{1/4} r_a^{-1/4} G_0, \quad \tilde{A} = r^{1/4} A r^{-1/4} \quad (11)$$

The equation for the causality Green's function G will be (12)

$$\begin{aligned} & [i\hbar \frac{\partial}{\partial s} + \frac{\hbar^2}{2m} (r \frac{\partial^2}{\partial r^2} + \frac{3}{2} \frac{\partial}{\partial r} + \frac{1}{r} \frac{\partial^2}{\partial \theta^2} + \frac{1}{r} \operatorname{ctg}\theta \frac{\partial}{\partial \theta} + \\ & + \frac{1}{r \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}) - V(r) - (\frac{\hbar^2}{2m}) \frac{3}{16r}] G = \\ & = i\hbar \delta(s_b - s_a) r_b^{-1/2} \sin^{-1} \theta_b \delta(r_b - r_a) \delta(\theta_b - \theta_a) \delta(\varphi_b - \varphi_a). \end{aligned} \quad (12)$$

Hence, using (10) and (11) we obtain the representations of the function G through the Green's function G . Let us now re-write the obtained relation as a relation between path integral symbols. It can be done, since the differential operators in (9) and (12) are a sum of Laplace-Beltrami operators and potentials. Consequently, the measures in the path integrals are identically determined with the help of stochastic processes given by stochastic differential equations with their local form being of the Stratonovich type

The path integral relation will be

$$\begin{aligned} & (r_a \sin^2 \theta_a)^{-1/4} (r_b \sin^2 \theta_b)^{-1/4} \int_{(r, \theta, \varphi)(s_a) = (r_a, \theta_a, \varphi_a)}^{(r, \theta, \varphi)(s_b) = (r_b, \theta_b, \varphi_b)} \frac{D(r, \theta, \varphi) D(p_r, p_\theta, p_\varphi)}{[2\pi\hbar]^3} \exp\left(\frac{i}{\hbar} \int_{s_a}^{s_b} [p_r r' + p_\theta \theta' + \right. \\ & \left. + p_\varphi \varphi' - \frac{1}{2m} (r p_r^2 + \frac{1}{r} p_\theta^2 + \frac{1}{r \sin^2 \theta} p_\varphi^2) - V(r) - (\frac{\hbar^2}{2m}) \frac{3}{16r}] ds\right) = \end{aligned}$$

$$\begin{aligned}
&= (r_a^{1/4} r_b^{1/4}) \frac{1}{16} \int_0^{4\pi} d\alpha_b (r_a^2 \sin^2 \theta_a)^{-1/4} (r_b^2 \sin^2 \theta_b)^{-1/4} \\
&\quad \int \frac{D(r, \theta, \varphi, \alpha) D(p_r, p_\theta, p_\varphi, p_\alpha)}{[2\pi\hbar]^4} \times \\
&\quad (r, \theta, \varphi, \alpha)(s_a) = (r_a, \theta_a, \varphi_a, \alpha_a) \\
&\quad (r, \theta, \varphi, \alpha)(s_b) = (r_b, \theta_b, \varphi_b, \alpha_b) \\
&\quad \times \exp\left(\frac{i}{\hbar} \int_{s_a}^{s_b} [p_r r' + p_\theta \theta' + p_\varphi \varphi' + p_\alpha \alpha' - \frac{1}{2m}(r p_r^2 + \frac{1}{r} p_\theta^2 + \frac{1}{r \sin^2 \theta} p_\varphi^2 + \right. \\
&\quad \left. + \frac{1}{r \sin^2 \theta} p_\alpha^2 + \frac{2 \cos \theta}{r \sin^2 \theta} p_\alpha p_\varphi - V(r)] ds\right). \tag{13}
\end{aligned}$$

By choosing $V(r) = v(r) - (\hbar^2/2m)3/16r$ due to the arbitrariness of the function $V(r)$, we may put the exponential part of the reduction Jacobian into the R.H.S. of (13). Afterwards we shall consider such a choice for $V(r)$ in formula (13) to be made.

An important remark following from formula (13) is that the realization of the reduction procedure in the path integral symbol, which is usually performed by substituting identities into the path integral and further transition from the repeated path integral to a multiple one, may lead us to the Jacobians different from identity. In our case

$$\begin{aligned}
&(r_a \sin^2 \theta_a)^{-1/4} (r_b \sin^2 \theta_b)^{-1/4} \left(\frac{D(r, \theta, \varphi) D(p_r, p_\theta, p_\varphi)}{[2\pi\hbar]^3} \right) \left(\frac{D_\alpha D p_\alpha}{[2\pi\hbar]} \right) = \\
&= (r_a^{1/4} r_b^{1/4}) (r_a^2 \sin^2 \theta_a)^{-1/4} (r_b^2 \sin^2 \theta_b)^{-1/4} \exp\left(\frac{i}{\hbar} \left(\frac{\hbar^2}{2m}\right) \int_{s_a}^{s_b} \left(\frac{3}{16r}\right) ds\right) \\
&\quad \left(\frac{D(r, \theta, \varphi, \alpha) D(p_r, p_\theta, p_\varphi, p_\alpha)}{[2\pi\hbar]^4} \right).
\end{aligned}$$

It should also be noted that contrary to a "discrete approach to the path integral" where the Jacobian exponential part (additional potential term) is interpreted as a quan-

tum correction term under the operator ordering, in our approach one may trace its relation with the geometry of the problem.

If one applies formula (13) to the path integral from (6) then it may be seen that in this the Jacobians arising from the reparametrization and reduction procedures, are mutually cancelled.

Finally, in order to relate the Green's function of hydrogen atom to the Green's function of four-dimensional harmonic oscillator, one has to make point transformations from the variables $(r, \theta, \varphi, \alpha)$ to the variables (u_1, u_2, u_3, u_4) . In the path integral symbol, the expression

$$\frac{1}{2\mu} \left(4r p_r^2 + \frac{4}{r} p_\theta^2 + \frac{4}{r \sin^2 \theta} p_\varphi^2 + \frac{4}{r \sin^2 \theta} p_\alpha^2 + \frac{8 \cos \theta}{r \sin^2 \theta} p_\alpha p_\varphi \right) - E r$$

will transform into

$$\frac{1}{2\mu} (p_1^2 + p_2^2 + p_3^2 + p_4^2) - E u^2.$$

due to the rule for the point transformation of the path integral symbol.

We have beforehand chosen $m=4\mu$ in the path integral. This choice has brought us to the appearance of the number factors in $g^{-1/4}(a)g^{-1/4}(b)$ of the path integral symbol, however the point transformation of the path integral removes these number factors.

As a result we come to the known relation between the Green's functions for hydrogen atom and four-dimensional harmonic oscillator (see /1/).

As for the one-dimensional case (the radial hydrogen atom problem) it should be noted that path integral transformations should be made in a similar way, but the only difference is that instead of Kustaanheimo-Stiefel transformation one should use a homogeneous point transformation.

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