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PATH INTEGRAL FOR SEPARABLE HAMILTONIANS OF LIOUVILLE-TYPE

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A general path-integral analysis of the separable Hamiltonian of Liouville-type is reviewed. The basic dynamical principle used is Jacobi's principle of least action for given energy which is reparametrization invariant, and thus the gauge freedom naturally appears. The choice of gauge in a path integral corresponds to the separation of variables in operator formalism. The gauge independence and the operator ordering are closely related. The path integral in this formulation sums over orbits in space instead of space-time. An exact path integral of the Green's function for the hydrogen atom in parabolic coordinates is illustrated as an example, which is also interpreted as a one-dimensional quantum gravity with a quantized cosmological constant.

1 Introduction

In 1979, Duru and Kleinert [1] showed an elegant path-integral method to exactly evaluate the Green's function for the hydrogen atom. Two basic ingredients in their method are the use of a re-scaled time variable and the so-called Kustaanheimo-Stiefel transformation [2] which reveals the $O(4)$ symmetry explicitly in the coordinate space. The physical meaning of the "re-scaled time variable" however remained somewhat unclear [3]. I have studied this issue by recognizing the procedure in Ref. [1] as a special case of the general treatment of the classically separable Hamiltonian of Liouville-type. The basic dynamical principle involved is then identified as Jacobi's principle of least action for given energy [4].

The path integral on the basis of Jacobi's principle of least action is basically static and analogous to geometrical optics, and one deals with a sum

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over orbits in *space* instead of space-time. Another characteristic of the Jacobi principle of least action is that it is reparametrization invariant. The general technique of gauge theory is thus applicable to the evaluation of a path integral, and a suitable choice of gauge simplifies the problem such as the hydrogen atom. A simple trick in parabolic coordinates, which was used before in a different context by Ravndal and Toyoda [5], renders the hydrogen atom Hamiltonian, a separable form of Liouville-type.

The hydrogen atom path integral is also understood as a one-dimensional quantum gravity; an interesting aspect of this picture is that the cosmological constant is *quantized* [6].

2 Separable Hamiltonian of Liouville-Type

We start with a separable Hamiltonian

$$H = \frac{1}{V_1(q_1)+V_2(q_2)}\left\{\frac{1}{2m}(p_1^2+p_2^2)+U_1(q_1)+U_2(q_2)\right\}, \tag{1}$$

where the variables vary over $\infty > q_1, q_2 > -\infty$. A general Hamiltonian of Liouville-type is given by

$$H = \frac{1}{V_1(Q_1)+V_2(Q_2)} \times\left\{\frac{1}{2mW_1(Q_1)}P_1^2+\frac{1}{2mW_2(Q_2)}P_2^2+U_1(Q_1)+U_2(Q_2)\right\}, \tag{2}$$

but after a canonical transformation

$$\begin{aligned}\frac{1}{\sqrt{W_1(Q_1)}}P_1 = p_1\ ,\ \int_0^{Q_1}\sqrt{W_1(Q)}dQ = q_1,\\ \frac{1}{\sqrt{W_2(Q_2)}}P_2 = p_2\ ,\ \int_0^{Q_2}\sqrt{W_2(Q)}dQ = q_2\end{aligned} \tag{3}$$

and a suitable redefinition of V and U, we can write the Hamiltonian in the form of (1).

We may then solve the Schrödinger problem

$$E\psi = \frac{1}{V_1(q_1)+V_2(q_2)}\left\{\frac{1}{2m}(\hat{p}_1^2+\hat{p}_2^2)+U_1(q_1)+U_2(q_2)\right\}\psi, \tag{4}$$

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where

$$\hat{p}_l = -i\hbar \frac{\partial}{\partial q_l} \tag{5}$$

for $l = 1, 2$, and where the volume element dV, which renders the Hamiltonian H in (4) Hermitian, is given by

$$dV = (V_1(q_1) + V_2(q_2))dq_1 dq_2. \tag{6}$$

The classical Hamiltonian (1) does not completely specify the operator ordering in (4), and the simplest ordering is adopted here. A precise operator ordering needs to be fixed depending on each explicit example.

One may rewrite the above Schrödinger equation (4) as

$$\hat{H}_T \psi = 0 \tag{7}$$

with a *total Hamiltonian* defined by a specific gauge condition,

$$\hat{H}_T = \frac{1}{2m}(\hat{p}_1^2 + \hat{p}_2^2) + U_1(q_1) + U_2(q_2) - E(V_1(q_1) + V_2(q_2)). \tag{8}$$

The meaning of the total Hamiltonian is clarified later. A general procedure to deal with a completely separated operator $\hat{H}_T$ is to consider an evolution operator for a parameter τ defined by

$$\begin{aligned}
&\langle q_{1b}, q_{2b}|e^{-i\hat{H}_T\tau/\hbar}|q_{1a}, q_{2a}\rangle \\
&= \left\langle q_{1b} \left| \exp\left[-\frac{i}{\hbar}\left(\frac{1}{2m}\hat{p}_1^2 + U_1(q_1) - EV_1(q_1)\right)\tau\right] \right| q_{1a} \right\rangle \\
&\quad \times \left\langle q_{2b} \left| \exp\left[-\frac{i}{\hbar}\left(\frac{1}{2m}\hat{p}_2^2 + U_2(q_2) - EV_2(q_2)\right)\tau\right] \right| q_{2a} \right\rangle \\
&= \int \mathcal{D}q_1 \mathcal{D}p_1 \exp\left[\frac{i}{\hbar}\int_0^\tau \left\{p_1\dot{q}_1 - \left(\frac{1}{2m}p_1^2 + U_1(q_1) - EV_1(q_1)\right)\right\} d\tau\right] \\
&\quad \times \int \mathcal{D}q_2 \mathcal{D}p_2 \exp\left[\frac{i}{\hbar}\int_0^\tau \left\{p_2\dot{q}_2 - \left(\frac{1}{2m}p_2^2 + U_2(q_2) - EV_2(q_2)\right)\right\} d\tau\right].
\end{aligned} \tag{9}$$

The parameter τ is arbitrary, and by integrating over τ from 0 to ∞ one obtains a physically meaningful quantity

$$\begin{aligned}
&\left\langle q_{1b}, q_{2b} \left| \frac{\hbar}{\hat{H}_T} \right| q_{1a}, q_{2a} \right\rangle_{\text{semi}-\text{classical}} \\
&\quad = i\int_0^\infty d\tau \frac{1}{\sqrt{2\pi i\hbar(\partial q_1(\tau)/\partial p_1(0))_{q_{1a}}}} \frac{1}{\sqrt{2\pi i\hbar(\partial q_2(\tau)/\partial p_2(0))_{q_{2a}}}}
\end{aligned}$$

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$$\times \exp\{(i/\hbar)S_{\rm cl}(q_{1b}, q_{1a}, \tau) + (i/\hbar)S_{\rm cl}(q_{2b}, q_{2a}, \tau)\}. \tag{10}$$

Here, the result is written as a semi-classical approximation for the path integral [7], though in certain cases one may be able to perform an exact path integral in (9). The prefactor in (10) is written in terms of classical paths, for example,

$$q_{1\rm cl}(\tau) = q_1(\tau; q_{1a}, p_1(0)). \tag{11}$$

This means that the classical paths, dictated by the total Hamiltonian $\hat{H}_T$, are expressed as functions of the initial positions and momenta. On the other hand, the classical action $S_{\rm cl}$ is expressed as a function of the initial position, the final position, and the elapsed "time" τ by eliminating, for example, the dependence on $p_1(0)$. Thus we obtain

$$S_{\rm cl}(q_{1b}, q_{1a}, \tau) = \int_0^\tau \left\{ p_1 \dot{q_1} - \left(\frac{1}{2m} p_1^2 + U_1(q_1) - E V_1(q_1) \right) \right\}_{\rm cl} d\tau \tag{12}$$

with $q_1(\tau) = q_{1b}$. If one solves the Hamilton-Jacobi equation in the form of

$$S(q_{1b}, q_{1a}; \tau) = -A\tau + S(q_{1b}, q_{1a}; A), \tag{13}$$

one treats A as a dynamical variable and regards the above equation as a Legendre transformation defined by

$$\begin{aligned} \frac{\partial S(q_{1b}, q_{1a}; \tau)}{\partial \tau} &= -A, \\ \frac{\partial S(q_{1b}, q_{1a}; A)}{\partial A} &= \tau. \end{aligned} \tag{14}$$

The variable A is then eliminated. This may be regarded as a classical analogue of the uncertainty relation; if one specifies τ, the conjugate variable A becomes implicit. It is well known that the semi-classical approximation (10) is exact for a quadratic system.

We next note the relation for the quantity defined on the left-hand side of (10):

$$\begin{aligned} &\left\langle q_{1b}, q_{2b} \left| \frac{1}{\hat{H}_T} \right| q_{1a}, q_{2a} \right\rangle \\ &\quad = \left\langle q_{1b}, q_{2b} \left| \frac{1}{\left(\frac{1}{\hat{V}_1(q_1) + \hat{V}_2(q_2)} \right) \hat{H}_T} \right| q_{1a}, q_{2a} \right\rangle \frac{1}{V_1(q_{1a}) + V_2(q_{2a})} \end{aligned}$$

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$$
\begin{aligned}
&= \left\langle q_{1b}, q_{2b} \left| \frac{1}{\hat{H} - E} \right| q_{1a}, q_{2a} \right\rangle \frac{1}{V_1(q_{1a}) + V_2(q_{2a})} \qquad (15)\\
&= \frac{1}{H\left(q_{1b}, \frac{\hbar}{i}\frac{\partial}{\partial q_{1b}}, q_{2b}, \frac{\hbar}{i}\frac{\partial}{\partial q_{2b}}\right) - E}\\
&\quad \times \left\{ \frac{1}{\sqrt{V_1(q_{1b}) + V_2(q_{2b})}} \langle q_{1b}, q_{2b} | q_{1a}, q_{2a} \rangle \frac{1}{\sqrt{V_1(q_{1a}) + V_2(q_{2a})}} \right\},
\end{aligned}
$$

by recalling $(\hat{A}\hat{B})^{-1} = \hat{B}^{-1}\hat{A}^{-1}$. The state vectors in these relations are defined for the volume element $dq_1 dq_2$ as

$$
\int dq_1 dq_2 |q_1, q_2\rangle\langle q_1, q_2| = 1. \qquad (16)
$$

Note that the definition of the δ-function in $\langle q_1', q_2'|q_1, q_2\rangle = \delta(q_1' - q_1)\delta(q_2' - q_2)$ depends on the choice of the volume element in (16) and thus on the choice of H_T. The last expression in (15) is thus correctly defined for the original Hamiltonian H and the original state ψ in (4) with the volume element dV in (6), since we have the completeness relation from (16)

$$
\int |q_1, q_2\rangle \frac{dV}{V_1(q_1) + V_2(q_2)} \langle q_1, q_2| = 1. \qquad (17)
$$

The left-hand side of (15) thus defines the correct Green's function for the original operator $(\hat{H} - E)^{-1}$ by noting the symmetry in q_a and q_b. One can then define the conventional evolution operator by

$$
\begin{aligned}
&\left\langle q_{1b}, q_{2b} \left| e^{-i\hat{H}(t_b - t_a)/\hbar} \right| q_{1a}, q_{2a} \right\rangle_{\text{conv}}\\
&\quad = \frac{1}{2\pi i\hbar} \int_{-\infty}^{\infty} dE e^{-iE(t_b - t_a)/\hbar}\\
&\qquad \times \left\langle q_{1b}, q_{2b} \left| \frac{\hbar}{\hat{H} - i\epsilon - E} \right| q_{1a}, q_{2a} \right\rangle \frac{1}{V_1(q_{1a}) + V_2(q_{2a})}, \qquad (18)
\end{aligned}
$$

where ϵ is an infinitesimal positive number. The total Hamiltonian changes by a different choice of gauge condition in Jacobi's principle of least action to be explained below. Consequently, the volume element, which renders H_T Hermitian, generally depends on the choice of gauge. In the present case, one has the relation

$\langle q_{1b}, q_{2b}|q_{1a}, q_{2a}\rangle_{\text{conv}}$

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$$= \langle q_{1b}, q_{2b}|q_{1a}, q_{2a}\rangle \frac{1}{V_1(q_{1a}) + V_2(q_{2a})}$$
$$= \frac{1}{\sqrt{V_1(q_{1b}) + V_2(q_{2b})}} \langle q_{1b}, q_{2b}|q_{1a}, q_{2a}\rangle \frac{1}{\sqrt{V_1(q_{1a}) + V_2(q_{2a})}}. \quad (19)$$

3 Jacobi's Principle of Least Action

The meaning of the total Hamiltonian H_T (8) becomes transparent if one starts with Jacobi's principle of least action for a given E,

$$S = \int_0^\tau d\tau L \quad (20)$$
$$= \int_0^\tau d\tau \sqrt{2m[E(V_1(q_1) + V_2(q_2)) - (U_1(q_1) + U_2(q_2))](\dot{q}_1^2 + \dot{q}_2^2)}$$
$$= \int \sqrt{2m[E(V_1(q_1) + V_2(q_2)) - (U_1(q_1) + U_2(q_2))][(dq_1)^2 + (dq_2)^2]},$$

which is reparametrization invariant. One then defines the momenta conjugate to coordinates

$$p_l = \frac{\partial L}{\partial \dot{q}_l} \quad (21)$$
$$= \sqrt{2m[E(V_1(q_1) + V_2(q_2)) - (U_1(q_1) + U_2(q_2))]} \times \frac{\dot{q}_l}{\sqrt{(\dot{q}_1^2 + \dot{q}_2^2)}}$$

and obtains a vanishing Hamiltonian as a result of reparametrization invariance. Furthermore we obtain a first class constraint ϕ as the generator of reparametrization gauge symmetry,

$$H = p_l\dot{q}_l - L = 0,$$
$$\phi(q_l, p_l) = \frac{1}{V_1(q_1) + V_2(q_2)} \left\{ \frac{1}{2m}(p_1^2 + p_2^2) + U_1(q_1) + U_2(q_2) \right\} - E$$
$$\simeq 0. \quad (22)$$

Following Dirac [8], one may then define a *total Hamiltonian*

$$H_T = H + \alpha(q_l, p_l)\phi(q_l, p_l) = \alpha(q_l, p_l)\phi(q_l, p_l) \simeq 0, \quad (23)$$

where an arbitrary function $\alpha(q_l, p_l)$ specifies a choice of *gauge* or a choice of the arbitrary parameter τ in (20), which parameterizes the orbit for a given

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E. The quantum theory is defined, up to an operator ordering, by

$$i\hbar\frac{\partial}{\partial\tau}\psi = \hat{H}_T\psi \tag{24}$$

with the physical state condition

$$\hat{\alpha}(q_l, p_l)\hat{\phi}(q_l, p_l)\psi_{phy} = 0. \tag{25}$$

The choice of the specific gauge $\alpha(q_l, p_l) = V_1(q_1) + V_2(q_2)$ gives rise to (7) and the choice $\alpha(q_l, p_l) = 1$ gives the conventional static Schrödinger equation (4), since ψ appearing in these equations are physical states.

The basic dynamical principle involved is thus identified as the Jacobi principle of least action, which is analogous to geometrical optics, and the formula for an evolution operator (9) dictated by (24) provides a basis for the path-integral approach to a general separable Hamiltonian of Liouville-type. The path integral in (9) deals with a sum over orbits in space instead of space-time, and the notion of re-scaled time does not explicitly appear in the present approach. The evolution operator (9) essentially generates a *gauge transformation*.

4 Hydrogen Atom

It is known that the Schrödinger equation for the hydrogen atom can be written in parabolic coordinates as

$$\begin{aligned}\hat{\tilde{H}}_T\psi &= 0,\\ (\hat{p}_\varphi - \hat{p}_{\varphi'})\psi &= 0,\end{aligned} \tag{26}$$

with the Hamiltonian

$$\begin{aligned}\hat{\tilde{H}}_T &= \frac{1}{2m}\left[\hat{p}_u^2 + \frac{1}{u^2}\hat{p}_\varphi^2 + \hat{p}_v^2 + \frac{1}{v^2}\hat{p}_{\varphi'}\right] + \frac{m\omega^2}{2}(u^2+v^2) - e^2\\ &= \frac{1}{2m}\vec{p}_u^{\,2} + \frac{m\omega^2}{2}\vec{u}^2 + \frac{1}{2m}\vec{p}_v^{\,2} + \frac{m\omega^2}{2}\vec{v}^2 - e^2,\end{aligned} \tag{27}$$

where we define

$$\begin{aligned}\vec{u} &= (u_1, u_2) = (u\cos\varphi, u\sin\varphi),\\ \vec{p}_u^{\,2} &= \hat{p}_u^2 + \frac{1}{u^2}\hat{p}_\varphi^2,\\ \vec{v} &= (v_1, v_2) = (v\cos\varphi', v\sin\varphi'),\end{aligned}$$

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$$\vec{p}_v^{\,2} = \hat{p}_v^2 + \frac{1}{v^2}\hat{p}_{\varphi'}^2. \tag{28}$$

The subsidiary condition (26) renders a quadratic Hamiltonian of Liouville-type for the hydrogen atom without recourse to the Kustaanheimo-Stiefel transformation [2]. This introduction of auxiliary variables (28) has been discussed by Ravndal and Toyoda [5].

The general procedure is thus applicable to the hydrogen atom, and we recover the classical exact result of Duru and Kleinert [1].

5 Quantum Gravity with a Quantized Cosmological Constant

An alternative way to see the physical meaning of the parameter τ is to study the one-dimensional quantum gravity coupled to matter variables $\vec{x}$, defined by

$$\int \frac{\mathcal{D}\vec{x}\mathcal{D}h}{\text{gauge volume}} \exp\left\{\frac{i}{\hbar}\int_0^\tau Lh\, d\tau\right\}, \tag{29}$$

with

$$L = \frac{m}{2h^2}\left(\frac{d\vec{x}}{d\tau}\right)^2 - V(r) + E, \tag{30}$$

where h stands for the einbein, a one-dimensional analogue of the vierbein h_μ^a, and $h = \sqrt{g}$ in one dimension. If one uses the solution of the equation of motion for h defined by the Lagrangian $\mathcal{L} = Lh$, the action in (29) is reduced to the one appearing in Jacobi's principle of least action. An interesting aspect of this interpretation is that one has a toy model of quantum gravity with a quantized cosmological constant [6].

6 Discussion

A method for exactly solving the Green's function for the hydrogen atom via path integrals [1] opened a new avenue for the path-integral treatment of a general separable Hamiltonian of Liouville-type. This new point of view, which has been shown to be based on Jacobi's principle of least action, provides a more flexible framework of path integrals to deal with a wider class of problems of physical interest. Jacobi's principle of least action, besides being reparametrization invariant, gives a geometrical picture of particle orbits in a

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curved space deformed by the potential. On the other hand, the fundamental space-time picture of the conventional Feynman path integral, which is associated with Hamilton's principle of stationary action, is lost.

I learned the path integral of the hydrogen atom through a seminar given by C. Bernido, who provided me with references to the work of Kleinert. Though I have spent much time on the path integral in relativistic quantum field theory, I wrote only two papers on path integrals of non-relativistic quantum mechanics. By publishing these papers [4,6], I was embarrassed to find an enormous difference of *culture* between physicists in relativistic and non-relativistic fields regarding path integrals; the major issue in the latter field of non-relativistic path integral is *operator ordering*, which is not fundamental in relativistic problems mainly due to the strong constraints provided by the symmetry principles such as Lorentz and gauge invariance. An over-emphasis on the operator ordering problem does not appear to be healthy.

I believe that a more fruitful field will open if the researchers in these two realms of path integrals work together. Professor H. Kleinert will certainly be one of the leaders in such an attempt.

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