Quantization in nonlinear coordinates via Hamiltonian path integrals

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Difficulties of using Hamiltonian path integrals as a method of quantization in nonlinear coordinates are discussed. It is shown that a straightforward generalization of Pauli-DeWitt configuration-space path integrals to canonical path integrals fails even for simple systems.

I. INTRODUCTION

The Feynman path-integral method is one of the most attractive alternatives to canonical quantization.[1] The central object of this formulation is the propagator

$$\langle q''\,|\exp[-iH(t''-t')/\hbar]\,|\,q'\rangle \equiv \langle q''t''\,|\,q't'\rangle \;.$$

It obeys the group property[2]

$$\langle q''t''\,|\,q't'\rangle = \int (dq)\langle q''t''\,|\,qt\rangle\langle qt\,|\,q't'\rangle \;. \tag{1}$$

Dividing the interval (t',t'') into n parts $t''>t_{n-1}>\cdots>t_1>t'$ and using the group property (1) one easily gets

$$\langle q''t''\,|\,q't'\rangle = \int (dq_1\cdots dq_{n-1})\langle q''t''\,|\,q_{n-1}t_{n-1}\rangle\langle q_{n-1}t_{n-1}\,|\,q_{n-2}t_{n-2}\rangle\cdots\langle q_1t_1\,|\,q't'\rangle \;. \tag{2}$$

The quantization proceeds by giving a prescription for the short-time propagator and using it in the right-hand side of Eq. (2). The path-integral representation for the propagator is obtained in the limit $n\to\infty$. It is well known that in order to avoid ambiguities in the definition both the normalization as well as the path for the short-time propagator must be specified.[3] We prefer the Pauli-DeWitt expression[4,5]

$$\langle q''t''\,|\,q't'\rangle_0 = \frac{1}{(2\pi\hbar i)^{-N/2}} g''^{-1/4} D^{1/2} g'^{-1/4} \exp[iS(q''t''\,|\,q't')/\hbar] \;, \tag{3}$$

where $S(q''t''\,|\,q't')$ is the action computed along a classical trajectory having end points q',t' and q'',t'' and D is the van Vleck determinant[6]

$$D = \det\left[(-1)^N \frac{\partial^2 S}{\partial q''^i \partial q''^j}\right] \;, \tag{4}$$

where N is number of degress of freedom.[2] If we approximate $\langle q''t''\,|\,q't'\rangle$ by the expression (3), Eq. (2) defines the path integral completely.

The Feynman path-integral approach to quantization is based on the Lagrangian formulation and is invariant under point transformations, hence the quantization can be done in any set of generalized coordinates. Although the usual Schrödinger approach to quantum mechanics rests on the Hamiltonian form of dynamics there does not exist a satisfactory Hamiltonian path-integral method of quantization. There has been considerable interest[7] in representations of canonical transformations in quantum mechanics, and Hamiltonian path integrals can provide a way of attacking this problem. The equivalence of the existing canonical path integrals[8,9] to the configuration-space path integrals has been demonstrated only in Cartesian coordinates.[10] A general proof of the equivalence of the two path-integral formalisms does not exist. Although the phase-space path integrals are widely used to quantize complex systems like singular Lagrangian field theories[11] and are believed to be superior to the Lagrangian functional integrals, they have an unsatisfactory feature,[12] viz., the Hamiltonian path integrals are not invariant under point transformations, let alone under a full set of canonical transformations. This awkward feature manifests itself in the fact that $H(q,p)$ appearing in the path integral

$$\langle q''t''\,|\,q't'\rangle = \int\int \mathscr{D}p\,\mathscr{D}q \exp\left[\frac{i}{\hbar}\int [p\dot{q} - H(q,p)]dt\right]$$

must differ from the classical Hamiltonian by terms which depend on the choice of canonical coordinates in phase space even for the simplest systems. Almost all papers[13] on this subject focus attention essentially on getting these extra terms from the usual Schrödinger formalism or from Lagrangian path integrals. In this paper our interest[9] is neither in discussion of these papers nor in making fresh attempts in this direction. *We would like to investigate if it is possible to use Hamiltonian path integrals to quantize a classical system in nonlinear coordinates* in a way which is invariant at least under point transformation and if possible under a full set of canonical transformations also. Thus the path integral must be based on the classical Hamiltonian formalism and must not assume any knowledge of Lagrangian path integrals or any other method of quantization.

II. CONSTRUCTING THE CANONICAL PATH INTEGRALS

We start by making some observations on the Pauli-DeWitt expression (3). It has the following interesting properties.

(i) The expression (3) is also the semiclassical approximation to the exact propagator. In some special cases it already gives the exact propagator.[4]

(ii) $S(q''t''\,|\,q't')$ appearing in the exponential is the generator of a classical canonical transformation taking $q(t')$ to $q(t'')$. The Pauli-DeWitt expression is also the semiclassical expression for the transformation matrix specifying the quantum analog[14] of the classical canonical transformation.

(iii) The approximate expression (3) obeys the group property (1) if the integral is computed in the stationary-phase approximation.[15]

Just as the Lagrangian path integral can be built by folding the short-time propagators, the Hamiltonian path integral can be built up from the short-time approximation to the matrix elements

$$\langle q\,|\,e^{-iH(t''-t')}\,|\,p\rangle \equiv \langle qt''\,|\,pt'\rangle$$

and

$$\langle pt''\,|\,qt'\rangle \equiv \langle p\,|\,e^{-iH(t''-t')}\,|\,q\rangle \ .$$

Then we would replace (3) by

$$\langle q''t''\,|\,q't'\rangle_0 = \int dp\,\langle q''t''\,|\,pt\rangle_0 \langle pt\,|\,q't'\rangle_0 \ . \tag{5}$$

Here we wish to investigate if the following assumptions can be used to generate the Hamiltonian path integral and hence to quantize the system:

$$\langle q''t''\,|\,p\tau\rangle_0 = \frac{1}{g''^{1/4}} D_{++}^{1/2} \exp[iS_{++}(q''t''\,|\,p\tau)/\hbar] \ , \tag{6}$$

$$\langle p\tau\,|\,q't'\rangle_0 = \frac{1}{g'^{1/4}} D_{--}^{1/2} \exp[iS_{--}(p\tau\,|\,q't')/\hbar] \ , \tag{7}$$

$$D_{++} = \det\left|\frac{\partial^2 S_{++}}{\partial q''\partial p}\right|, \quad D_{--} = \det\left|\frac{\partial^2 S_{--}}{\partial q'\partial p}\right| \ .$$

Here p,q'' are the values of momenta and coordinates at the two ends of a trajectory between times τ and t'' ($t''>\tau$), and S_{++} is the generator of canonical transformation taking $p(\tau)$ to $q(t'')$. S_{--} is similarly defined.

The expressions (6) and (7) have properties similar to the properties of the Pauli-DeWitt formula (4) mentioned at the beginning of the section; for example, (6) and (7) share the property (ii). In addition, Eq. (5) gives the Pauli-DeWitt formula for $\langle q''t''\,|\,q't'\rangle_0$ when Eqs. (6) and (7) are used and the p integrals are calculated in the stationary-phase approximation. It is easily checked, using appropriate generalizations of Eqs. (9) and (10) of the next section, that the usual phase-space path integral

$$\int \mathscr{D}p\,\mathscr{D}q \exp\left[\frac{i}{\hbar}\int (p\dot{q}-H)dt\right] \tag{8}$$

results if we keep only first-order terms in $t''-\tau$ and $\tau-t'$ in Eqs. (6) and (7). It is, therefore, expected that the assumptions (6) and (7) are good candidates for generating canonical path integrals. This expectation is, however, not borne out. As we will show, by means of a simple example of a free particle in two dimensions using polar coordinates, the propagator based on Eq. (6) does not obey the correct Schrödinger equation. This result is quite surprising and it is not clear why quantization based on (6) and (7) fails to be equivalent to the usual Schrödinger equation.

It is of interest to note that in the nth-order approximation the paths in configuration space contributing to the propagator are specified as follows:

(i) Subdivide the interval $(t'-t'')$ into $n+1$ parts $t''>t_n>\cdots>t_1>t'$.

(ii) At each intermediate time t_k, value of coordinates are fixed at q_k. The path in the time interval (t_k,t_{k+1}) is taken to be the classical trajectory joining q_k and q_{k+1}. It must be noticed that the momenta will, in general, be discontinuous at times $t_1,\ldots,t_n$.

(iii) The intermediate values q_k, $k=1,\ldots,N$, are allowed to take all possible values.

Our assumptions (6) and (7) correspond to the phase-space paths described in the nth-order approximation by specifying values of q's and p's at alternate times, and the path in any one time interval is a classical trajectory with specified values of coordinates q at one end point and of momenta at the other end point. Of course now momenta and coordinates will be discontinuous for the path so specified at alternate intermediate times.

III. FREE PARTICLE IN TWO DIMENSIONS

We now consider a free particle in two dimensions using polar coordinates. We construct the first-order approximation to the path integral using Eqs. (5)–(7). We will show that the discrepancy between the equation obeyed by the first-order approximate expression and the correct Schrödinger equation does not go to zero as $t'\to t''$.

To get the first-order approximation subdivide the time interval (t',t'') into two parts (t',τ) and (τ,t'') by introducing an intermediate time τ. Let Γ_1 and Γ_2 be the classical trajectories followed during the two intervals (t',τ) and (τ,t''), respectively, when coordinates are held fixed at extreme points and the momenta have values at intermediate time τ as specified below:

$$t=t',\quad q'=(r',\theta') \ ,$$

$$t=\tau,\quad p=(p_r,p_\theta) \ ,$$

$$t=t'',\quad q''=(r'',\theta'') \ .$$

In general the q's will not be continuous at time $t=\tau$. Let values of (r,θ) at time τ for the two trajectories Γ_1 and Γ_2 be (r_1,θ_1) and (r_2,θ_2), respectively. Then $S_{\pm\pm}$ (Ref. 16) are Legendre transforms of the classical action for the two trajectories

$$S_{++}(q''t''\,|\,p\tau)=p_r r_2+p_\theta\theta_2+\int_{\Gamma_2}L\,dt\ , \tag{9}$$

$$S_{--}(p\tau\,|\,q't')=-p_r r_1-p_\theta\theta_1+\int_{\Gamma_1}L\,dt\ . \tag{10}$$

Using the equations of motion, r_1,θ_1 and r_2,θ_2 and the two integrals can be expressed as power series in $\delta\equiv\tau-t'$ and $\epsilon=t''-\tau$. After some straightforward computation we get

$$S_{++}(r''\theta''t''\,|\,p_r p_\theta\tau)=p_r r''+p_\theta\theta''-\epsilon\left[\frac{p_r^2}{2m}+\frac{p_\theta^2}{2mr''^2}\right]-\epsilon^2\frac{p_r p_\theta^2}{2mr''^3}+\epsilon^3\left[\frac{3}{2}\frac{p_r^2p_\theta^2}{m^3r''^4}-\frac{1}{6}\frac{p_\theta^4}{m^3r''^6}\right]+\cdots \tag{11}$$

and

$$S_{--}(p_r,r,\tau\,|\,r',\theta',t')=-p_r r'-p_\theta\theta'-\delta\left[\frac{p_r^2}{2m}+\frac{p_\theta^2}{2mr'^2}\right]+\frac{\delta^2}{2}\frac{p_r p_\theta^2}{m^2r'^3}+\delta^3\left[\frac{3}{2}\frac{p_r^2p_\theta^2}{m^3r'^4}-\frac{1}{6}\frac{p_\theta^2}{m^3r'^6}\right]+\cdots\ . \tag{12}$$

The terms proportional to ϵ^3 and higher are not important for our discussion below.[17] Computing D_{++} and D_{--} we have

$$D_{++}=\left[1+\tfrac{3}{2}\epsilon^2\frac{p_\theta^2}{m^2r''^4}\right],\quad D_{--}=\left[1+\tfrac{3}{2}\delta^2\frac{p_\theta^2}{m^2r'^4}\right].$$

Therefore, we have

$$\langle q''t''\,|\,q't'\rangle_0=\int\frac{dp_r dp_\theta}{(2\pi h)^2}\mathcal{K}\ , \tag{13}$$

where

$$\mathcal{K}=\frac{1}{(r'r'')^{1/2}}(D_{++}D_{--})^{1/2}\exp\left[\frac{i}{\hbar}(S_{++}+S_{--})\right]. \tag{13'}$$

Using the Hamilton-Jacobi equation for S_{++},

$$\frac{\partial S_{++}}{\partial t}+H_{\rm cl}\left[\frac{\partial S_{++}}{\partial q''},q''\right]=0\ ,$$

we get

$$i\hbar\frac{\partial}{\partial t''}\mathcal{K}=\left[\frac{1}{2m}\left[\frac{\partial S_{++}}{\partial r''}\right]^2+\frac{1}{2mr''^2}\left[\frac{\partial S_{++}}{\partial\theta''}\right]^2\right]+\frac{i\hbar}{2}\frac{\partial}{\partial t''}\ln D_{++}\ . \tag{14}$$

Also

$$\begin{aligned}\nabla_{r''}^2\mathcal{K}&=\left[\frac{\partial^2}{\partial r''^2}+\frac{1}{r''}\frac{\partial}{\partial r''}\frac{1}{r''^2}+\frac{\partial^2}{\partial\theta''^2}\right]\mathcal{K}\\&=\frac{1}{(r'r'')^{1/2}}\left[\frac{\partial^2}{\partial r''^2}+\frac{1}{r''^2}\frac{\partial^2}{\partial\theta''^2}+\frac{1}{4r''^2}\right](D_{++}D_{--})^{1/2}\exp\left[\frac{i}{\hbar}(S_{++}+S_{--})\right].\end{aligned}$$

Therefore,

$$-\frac{\hbar^2}{2m}\nabla_{r''}^2\mathcal{K}=\left[-\frac{1}{2m}\left[\frac{\partial S_{++}}{\partial r''}\right]^2-\frac{i\hbar}{2m}\frac{\partial^2S_{++}}{\partial r''^2}-\frac{1}{2m}\frac{1}{r''^2}\left[\frac{\partial S_{++}}{\partial\theta''}\right]^2+\frac{\hbar^2}{8mr''^2}\right]\mathcal{K}+\cdots\ . \tag{15}$$

Therefore,

$$i\hbar\frac{\partial\mathcal{K}}{\partial t}+\frac{\hbar^2}{2m}\nabla_{r''}^2\mathcal{K}=\left[\frac{i\hbar}{2}\frac{\partial}{\partial\epsilon}\ln D_{++}+\frac{i\hbar}{2m}\frac{\partial^2S_{++}}{\partial r''^2}+\frac{\hbar^2}{8mr''^2}\right]\mathcal{K}+O(\sqrt{\epsilon})\ . \tag{16}$$

Using the explicit expressions for D_{++} and S_{++} the first two terms cancel in the lowest important order in ϵ. Retaining only terms of first order in ϵ in the exponential of $\mathscr{K}$ and integrating over p_r, p_θ gives[18]

$$\left[i\hbar\frac{\partial}{\partial t''}+\frac{\hbar^2}{2m}\nabla_{r''}{}^2\right]\langle q''t''\,|\,q't'\rangle_0 = \frac{\hbar^2}{8mr''^2}\langle q''t''\,|\,q't'\rangle_0+O(\sqrt{\epsilon})\ . \quad (17)$$

It is, therefore, seen that the propagator so constructed will obey the equation

$$i\hbar\frac{\partial}{\partial t}K=(\hat{H}_0+V_{\text{eff}})K\ , \quad (18)$$

where

$$H_0=-\frac{\hbar^2}{2m}\nabla^2\ ,$$
$$V_{\text{eff}}=\frac{\hbar^2}{8mr^2}\ , \quad (19)$$
$$K\equiv\langle q''t''\,|\,q't'\rangle\ ,$$

which differs from the Schrödinger equation by the V_{eff} term. Hence in order that K may satisfy the correct Schrödinger equation, one must not use the classical Hamiltonian H_{cl}; instead $H_{\text{cl}}-V_{\text{eff}}$ must be used to construct the generators S_{++} and S_{--}. By any such *ad hoc* addition of V_{eff} to H_{cl} requires knowledge of the Schrödinger equation and defeats the original objective of formulating canonical path integrals entirely in terms of classical phase-space formalism quantities without assuming any knowledge of quantum mechanics.

V. CONCLUDING REMARKS

It must be emphasized here that although the operator representing the Hamiltonian in general nonlinear coordinates has ordering problems, in the example chosen above we do not have any of these problems because the classical Hamiltonian

$$H_{\text{cl}}=p_r{}^2/2m+p_\theta{}^2/2mr^2$$

gives a unique operator

$$\hat{H}=\hat{p}_r{}^2/2m+\hat{p}_\theta{}^2/2mr^2\ , \quad (20)$$

assuming that the correspondence between phase-space functions and operators is a linear one.

The difficulty encountered in the Hamiltonian path integrals is certainly not due to anything inherent in the path-integral formalism, because the same difficulties appear when we attempt to use canonical quantization in the nonlinear coordinates directly. The canonical quantization in r,θ directly should proceed by taking H as in Eq. (20) where the operators $\hat{p}_r$, $\hat{p}_\theta$, $\hat{r}$, $\hat{\theta}$ must obey canonical commutation relations

$$[\hat{r},\hat{p}_r]=i\hbar,\ \ [\hat{\theta},\hat{p}_\theta]=i\hbar\ .$$

The representation of the operators $\hat{p}_r$, $\hat{p}_\theta$ is

$$\hat{p}_r=i\hbar\frac{\partial}{\partial r}+\frac{i\hbar}{2r},\ \ \hat{p}_\theta=i\hbar\frac{\partial}{\partial\theta}\ . \quad (21)$$

The expression (21) when substituted in (20) gives

$$H=-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{1}{4r^2}\right]-\frac{\hbar^2}{2mr^2}\frac{\partial^2}{\partial\theta^2}$$
$$=-\frac{\hbar^2}{2m}\nabla^2+\frac{\hbar^2}{8mr^2}\ ,$$

which is precisely the operator $\hat{H}_0+V_{\text{eff}}$ appearing in Eq. (18). This clearly shows that the problem of K not satisfying the correct Schrödinger equation is independent of the problems of the functional-integral formalism or the factor-ordering problems of defining quantum-mechanical operators as long as the correspondence rule used is linear.

It may be remarked that though Eqs. (6) and (7) are natural generalizations of Pauli-DeWitt expressions, there is nothing sacrosanct about these expressions. One may attempt to modify the assumptions (6) and (7) by changing the normalization factor. If we multiply the right-hand sides of (6) and (7) by a function f then we must have

$$f\simeq 1+O(\epsilon^2)+O(\delta^2)$$

as the terms linear in ϵ,δ can be absorbed as terms independent of ϵ,δ in the Hamiltonian. Then it is certainly possible to adjust f so that the correct equation is obeyed for the example of Sec. V. However, a function f with simple form which could be generalized to arbitrary coordinates in higher dimensions was not found. This point, we believe, does not merit further discussion.

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[2] We suppress the index on generalized coordinates $q^{(1)},\ldots,q^{(N)}$ corresponding to the N different degrees of freedom. Also (dq) denotes the volume element $g^{1/2}dq^{(1)}\cdots dq^{(N)}$.

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[9] The terms phase-space path integrals, canonical path integrals, and Hamiltonian path integrals will refer to functional integrals of the type discussed in Refs. 8 and 10. We shall not discuss path integrals of the type introduced by other authors, for example, of Ref. 18.

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[17]It must be emphasized here that terms of the order ϵp_θ^2, etc., contribute a nonzero value in the limit $\epsilon \rightarrow 0$ after integrations have been carried out. For purposes of counting powers of ϵ in (16) the momenta must be taken to be of order $1/\sqrt{\epsilon}$. This is so because in the Gaussian integral the range of the values of momenta contributing significantly is of order $1/\sqrt{\epsilon}$.

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