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Quantization in Quantum System with Time-Dependent Boundary Condition

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An approach to quantize a quantum mechanical system with time-dependent boundary condition is proposed in the framework of canonical quantization. It can be achieved by introducing the time-dependent boundary condition into the usual Lagrangian. We set up the effective Hamiltonian formalism and believe that this formalism can provide a generalized method to calculate the boundary effects.

1. INTRODUCTION

In quantum physics, there has been much works [1–5] on nonlocal effects in quantum mechanical systems with time-dependent boundary conditions. Considerable progress in the understanding of these problems has been achieved, but there has not been sufficient analysis of the boundary effects of the system in the framework of canonical quantization. This quantization framework was developed on the basis that the quantum system persists to the classical limit in spite of the existence of quantum effects [6], and in application to time-dependent systems has been proved to be very convenient and adequate. The main aim of this paper is the investigation of nonlocal effects in quantum mechanics. We consider the problem from the canonical point of view on the evolution and quantization of a system with time-dependent boundary conditions in the framework of canonical quantization.

The actual boundary effect considered is extremely simple. It consists of a particle of mass *m* in a one-dimensional box. Thus the particle can be

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considered to be localized within the interior of the box, far from the walls. If, now, one wall of the box is moved, namely the box grows wider or narrower, the wave functions will grow or shrink accordingly, since it must vanish at the walls. As analyzed by Greenberger [4] for the same system, the wall motion will cause the change of the original Hamiltonian to an effective one, and therefore the particle wave function experiences a corresponding change. Here, we will start from the Hamilton equation of the particle motion (i.e., the Euler equation), and then by the usual action principle give the system Lagrangian. This Lagrangian can help us set up the effective Hamiltonian and construct the Schrödinger equation. It is demonstrated that, in the new canonical representation, a harmonic oscillator potential appears in such an effective Hamiltonian which depends on the boundary motion. Finally, the solutions of the Schrödinger equation are calculated.

2. LAGRANGIAN FORMALISM AND CANONICAL QUANTIZATION

For a particle inside an infinite square well with a moving wall, the potential is $V(q) = 0$ for $q \leq a_0$ and $V(q) = \infty$ otherwise, where a_0 is the width of the well. The original Hamiltonian of the particle in this well takes the form $\hat{H}_0 = \hat{p}^2/2m$, where $\hat{p}$ is the momentum operator. As usual, the quantum state of the particle is described by the wave function $\Phi(q, t)$, which is governed by the Schrödinger equation $i\hbar\dot{\Phi} = \hat{H}_0\Phi$ subject to the boundary condition $\Phi(q = 0, t) = 0 = \Phi(q = a_0, t)$. The normalized solutions to this equation and the Hamiltonian eigenvalues are

$$\Phi_l(q, t) = \sqrt{\frac{2}{a_0}} \sin\left(\frac{l\pi q}{a_0}\right), \qquad E_{0l} = \frac{\hbar^2 l^2 \pi^2}{2ma_0^2}, \qquad l = 1, 2, 3, \ldots \tag{1}$$

If now the width of the box is variable, so that $a_0 \to a = a(t)$, then the Schrödinger equation is unchanged, but the boundary condition $\Phi(q = 0, t) = 0 = \Phi(q = a_0, t)$ becomes time dependent,

$$\Phi(q = 0, t) = 0 = \Phi(q = a(t), t) \tag{2}$$

and so we must solve the same equation endowed with this new condition. According to the naive determination of the partial time derivative used in the Schrödinger equation, the new equation can be clarified by the following expression [4, 5]:

$$i\hbar\dot{\Phi} = \frac{[\hat{p} - (e/c)\mathbf{A}(\hat{q})]^2}{2m}\Phi \tag{3}$$

with the Hamiltonian $\hat{H} = (1/2m)[\hat{p} - e\mathbf{A}(\hat{q})/c]^2$, which can be understood as the effective Hamiltonian for the interaction between a particle of charge e and the electromagnetic field due to the vector potential $\mathbf{A} = -(mc\dot{a}/ae)\hat{q}$. By the quantum–classical correspondence between the dynamical equation for quantum operators and classical dynamical variables, $\hat{H}$ can also be expressed in the classical form [6]

$$H = \frac{[p - (e/c)\mathbf{A}(q)]^2}{2m} = \frac{p_c^2}{2m} \tag{4}$$

This Hamiltonian gives the canonical momentum of q by $p_c = m\dot{q} + mq\dot{a}/a$. So we have the Hamilton equation of the particle motion

$$\dot{p}_c = m\ddot{q} + m\frac{\ddot{a}}{a}q - m\frac{\dot{a}^2}{a^2}q + m\frac{\dot{a}}{a}\dot{q} = \frac{\partial H}{\partial q} = 0 \tag{5}$$

which can reproduce the Euler equation of the system [6]

$$m\frac{a}{a_0}\ddot{q} + m\frac{\ddot{a}}{a_0}q - m\frac{\dot{a}^2}{a_0 a}q + m\frac{\dot{a}}{a_0}\dot{q} = 0 \tag{6}$$

We find this Euler equation is compatible with a new effective Lagrangian

$$L_{\text{eff}} = \frac{a}{2a_0}m\dot{q}^2 + \frac{\dot{a}}{2a_0}m\dot{q}q - m\frac{\ddot{a}}{4a_0}q^2 + m\frac{\dot{a}^2}{2a_0 a}q^2 \tag{7}$$

which is obtained by introducing the time-dependent boundary condition $a = a(t)$ into the original one $L_0 = \frac{1}{2}m\dot{q}^2$.

In order to start the canonical procedure, it is convenient to introduce the canonical variables [6]

$$Q = \sqrt{\frac{a}{a_0}}\,q, \qquad P = \frac{\partial L_{\text{eff}}}{\partial \dot{Q}} \tag{8}$$

In Q coordinate, the effective Lagrangian (7) can be expressed in the form

$$L_{\text{eff}} = \frac{P^2}{2m} - V_{\text{eff}}(Q) \tag{9}$$

with the canonical momentum and potential energy

$$P = m\dot{Q} = m\sqrt{\frac{a}{a_0}}\,\dot{q} + m\frac{\dot{a}}{2\sqrt{aa_0}}q, \qquad V_{\text{eff}} = \frac{\ddot{a}}{4a}mQ^2 - \frac{3\dot{a}^2}{8a^2}mQ^2 \tag{10}$$

Thus, we obtain the effective Hamiltonian in the new representation (Q, P)

$$H_{\text{eff}} = P\dot{Q} - L_{\text{eff}} = \frac{P^2}{2m} + V_{\text{eff}}(Q) \tag{11}$$

Note that, if we understand the factor $\omega(t) = \sqrt{\ddot{a}/(2a) - 3\dot{a}^2/(4a^2)}$ as a time-dependent angular frequency, $V_{\text{eff}}(Q) = m\omega(t)^2Q^2/2$ describes a harmonic oscillatory potential. So $H_{\rm eff}(P, Q)$ represents the Hamiltonian of the time-dependent oscillatory system. As an example, we here consider the special case that one of the potential walls oscillates with frequency $2\omega_0$ harmonically, namely

$$a(t) = a_0\, e^{i2\omega_0 t} \tag{12}$$

Then the effective potential becomes $V_{\rm eff}(Q) = m\omega_0^2 Q^2/2$, with angular frequency ω_0, so that Eq. (11) represents a linear harmonic oscillator, which in the operator form is given by

$$\hat{H}_{\rm eff} = \frac{\hat{P}^2}{2m} + \frac{1}{2} m\omega_0^2\, \hat{Q}^2 \tag{13}$$

Now we can quantize the system by using the canonical quantization method with the commutators

$$[\hat{Q}, \hat{P}] = i\hbar, \qquad [\hat{Q}, \hat{Q}] = [\hat{P}, \hat{P}] = 0 \tag{14}$$

These commutation relations hold all the time in the Q representation.

3. SCHRÖDINGER EQUATION AND ITS SOLUTIONS

We have obtained an effective Hamiltonian that depends on the motion of the geometrical boundary, so that, when the boundary condition becomes stationary (i.e., $\dot{a} = 0$), we come back to $\hat{H}_0$. When the width of the box is variable, the canonical framework holds, and the Schrödinger equation governing the system evolution in the Q representation is

$$\left[i\hbar \frac{\partial}{\partial t} - \hat{H}_{\rm eff} \right] \Psi(Q, t) = 0 \tag{15}$$

endowed with boundary condition

$$\Psi(Q = 0, t) = 0 = \Psi(X = D = \sqrt{a/a_0}\, a, t) \tag{16}$$

In comparison with solving this equation directly in the q representation, it is rather easy to solve it in the Q representation. For a linear harmonic oscillator with angular frequency ω_0, the Schrödinger eigenvalue equation reads

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(Q)}{dQ^2} + \frac{1}{2} m\omega_0^2\, Q^2\, \Psi(Q) = E\Psi(Q) \tag{17}$$

To solve this equation, we first consider the condition that the particle energy is much smaller than the effective potential at the boundary, i.e., $E \ll V_{\rm eff}(D)$. In this case, the boundary condition $\Psi(Q = D) = 0$ can always be satisfied.

Thus that the normalized linear harmonic oscillator eigenfunctions are given by

$$\Psi_n(Q) = \left(\frac{\alpha}{2^{n-1}\sqrt{\pi}n!}\right)^{1/2} \exp\left(\frac{-\xi^2}{2}\right) H_n(\xi), \qquad n = 1, 3, 5, \ldots \tag{18}$$

where the quantum number n is a positive odd integer, the functions $H_n(\xi)$ are polynomials of order n, $\xi = \alpha Q$, and $\alpha = (m\omega_0/\hbar)^{1/2}$. Thus the system of the linear harmonic oscillator has the energy spectrum

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega_0 \tag{19}$$

Using Eq. (18), we have the expectation values of Q and P as follows:

$$\langle Q\rangle = \frac{\sqrt{n}}{\alpha}, \qquad \langle Q^2\rangle = \left(n + \frac{1}{2}\right) \frac{\hbar}{m\omega_0} \tag{20}$$

$$\langle P\rangle = \frac{m\omega_0\sqrt{n}}{\alpha}, \qquad \langle P^2\rangle = \left(n + \frac{1}{2}\right) m\hbar\omega_0 \tag{21}$$

Thus, in the case of a minimum wave packet in the Q representation, the mean square values of the coordinate and momentum variables are, respectively,

$$(\Delta Q)^2 = \frac{\hbar}{2m\omega_0}, \qquad (\Delta P)^2 = \frac{m\hbar\omega_0}{2} \tag{22}$$

The value of the uncertainty product $\Delta Q\Delta P$ at a definite instant of time ($t =$ 0) is given by $\Delta Q\ \Delta P = \hbar/2$. Writing $\psi(Q) = \Psi(Q, t = 0)$, we have [7]

$$\left(-i\hbar \frac{d}{dQ} - \langle P\rangle\right)\psi(Q) = \frac{2i(\Delta P)^2}{\hbar} (Q - \langle Q\rangle)\psi(Q) \tag{23}$$

With the help of Eqs. (20) and (21), we can integrate this first-order differential equation to give the minimum-uncertainty wave function

$$\psi(Q) = C \exp\left(\frac{im\omega_0\sqrt{n}}{\hbar\alpha} Q\right) \exp\left(-\frac{m\omega_0}{2\hbar} \left(Q - \frac{\sqrt{n}}{\alpha}\right)^2\right) \tag{24}$$

where C is a normalization constant.

Now, let us suppose that the effective potential $V_{\text{eff}}(Q)$ can be considered to be a small perturbation term for free-article movement in the Q representation; then, in the frame of ordinary perturbation theory, the eigenfunctions of the effective Hamiltonian and the eigenvalues are

$$\Psi_l(Q, t) = \Psi_l^{(0)} + \Psi_l^{(1)} + \ldots, \qquad l = 1, 2, 3, \ldots \tag{25}$$

$$E_l = E_l^{(0)} + E_l^{(1)} + \ldots \tag{26}$$

where

$$\Psi_l^{(0)} = \sqrt{\frac{2}{D}} \sin\left(\frac{l\pi}{D} Q\right), \qquad E_l^{(0)} = \frac{\hbar^2 l^2 \pi^2}{2mD^2} \tag{27}$$

are the normalized eigenfunctions and eigenvectors for the Hamiltonian

$$\hat{H}_0(Q) = -\frac{\hbar^2}{2m} \frac{d^2}{dQ^2}$$

The first-order corrections $\Psi_l^{(1)}$ and $E_l^{(1)}$ are expressed as

$$\Psi_l^{(1)} = \frac{4m\omega_0 D^2}{\hbar\pi^2} \sum_k \frac{kl \cos(k\pi) \cos(l\pi)}{(k - l)(k^2 - l^2)^2} \Psi_k^{(0)}, \qquad k \neq l \tag{28}$$

$$E_l^{(1)} = \frac{2l^2\pi^2 - 3}{12l^2\pi^2} m\omega_0^2 D^2 = \frac{2l^2\pi^2 - 3}{6l^2\pi^2} V_{\text{eff}}(D) \tag{29}$$

It is obvious that, as $\dot{a} = 0$, $\Psi_l^{(0)} \to \Phi_l(x, t)$, $E_l^{(0)} \to e_l$, and $\Psi_l^{(1)} = E_l^{(1)} = 0$. This is an example of applying canonical quantization to a quantum mechanical system with a time-dependent boundary condition. The method can be extended to the three-dimensional case.

4. SUMMARY

A method to quantize a quantum mechanical system with a nonstationary boundary in the framework of canonical quantization was presented. We started from a time-dependent Hamiltonian in a quantum mechanical system with nonstationary boundary conditions and then gave the corresponding effective Lagrangian, which can be obtained by introducing the boundary effect into the original one. Furthermore, the effective Hamiltonian of the system was constructed in a new representation which represents nothing but the harmonic oscillator, and using it allowed us directly to apply to the system itself the standard procedures of quantization. The solutions of the Schrödinger equation (15) were calculated, and should be equivalent to those of $i\hbar\dot{\Phi} = \hat{H}_0\Phi$ with time-dependent boundary condition.

Finally, we believe that the presented formalism not only can be used to calculate the boundary effects, but also work within the region where the interaction between the system and environment is considered. Once the connection of the system with the environment is examined, the factor $\sqrt{a/a_0}$ in the effective Hamiltonian can be replaced by a time-dependent function reflecting the environment's effect on the system. In principle, it should be derived from the investigation of the dynamics of the system–environment connection.

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