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Geometrical Treatment of Nonholonomic Phase in Quantum Mechanics and Applications

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We discuss the description of quantum mechanical systems with Hamiltonians depending on slowly varying parameters by means of fiber bundles. A new Heisenberg equation is obtained. The problem of particle creation is treated through Berry's connection. We consider also a particle in a well with a moving wall. This system is equivalent to a particle interacting with a vector field dependent on the coordinate and relative velocity of the wall. The geometrical phase in this case is found.

1. INTRODUCTION

In recent years much attention has been paid to classical and quantum dynamical systems with variable parameters. Such tasks are typical in many areas of physical investigation, for example, particle creation and annihilation in strong external fields, dynamical systems characterized by "slow" and "fast" variables, and systems with nonstationary boundary conditions. As a rule, such problems are not exactly soluble. Special methods have been proposed to study these problems—the "averaging" method in classical mechanics, and the adiabatic (WKB) approximation in quantum mechanics. The last is based on the Born–Fock hypothesis (Born and Fock, 1928) and Ehrenfest's theorems (Ehrenfest, 1959).

Analyses of these old problems (Berry, 1984; Simon, 1983; Hannay, 1985) led to a new evolutionary picture of classical and quantum physical systems with slowly changing parameters. In the simplest understanding of the adiabatic hypothesis, any state of a dynamical system should transit to

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the state with the same quantum numbers in the case of an adiabatic variation of parameters (Messiah, 1981). Berry showed that when the Hamiltonian depends on several parameters that change adiabatically with time, there is another contribution to the phase factor acquired by the wave function of the system. This new phase is defined only by the geometry and topology of the parameter manifold. There are many physical effects due to this phase, among them the rotation of the polarization plane of a light beam (Tomita and Chiao, 1986) and the energy level shift in diatoms (Mead and Truhlar, 1979).

The analogous result for classical evolution was found by Hannay (1985) for the generalized harmonic oscillator in "action–angle" variables. The geometrical interpretation of topological phase was proposed first by Simon (1983).

Numerous papers devoted to the interpretation and calculation of Berry's (topological) phase, Berry's connection (see, for example, Jackiw, 1988), and curvature have advanced our understanding of the phenomenon. Elegant mathematical work (Asch, 1990; Buslaev, 1988; Kiritsis, 1987; Montgomery, 1988) has made it possible to classify a $U(1)$ connection. The adiabatic restriction on changing parameters was eliminated in recent work (Anandan and Aharonov, 1988; Wong, 1990). Moreover, noncyclic evolution was investigated (Zak, 1989). But it is necessary to remark that problems connected with the geometrical and topological properties of state space were not studied.

Now it is useful to combine the evolutionary picture with geometrical methods. The previous results were discussed by Uhlmann (1989) and Arodz and Babinch (1989). We believe that many well-known phenomena (breakdown of symmetry, particle creation, etc.) can be treated in geometrical phase terms.

This paper is devoted only to a small part of the problems connected with the Heisenberg equations for operators of physical variables and to a consideration of some physical and geometrical aspects of the dynamics of quantum mechanical systems with changing parameters and nonstationary boundary conditions.

In the next section we give a geometrical treatment of the Schrödinger equation and describe the essential points of our considerations.

Section 3 is devoted to the problem of Berry's phase removability. The appearance of Berry's phase, the particle creation problem, and effective Hamiltonians are discussed in Section 4.

Section 5 is devoted to an expansion of Berry's phase ideology to systems with time-dependent boundary conditions.

Finally, Section 6 contains some conclusions.

2. FIBER BUNDLES AND QUANTUM MECHANICS

2.1. States and Operators

Let us consider a quantum mechanical system governed by the Hamiltonian operator $\mathbf{H}$. We assume that $\mathbf{H}$ is a time-independent operator and time-independent boundary conditions are applied on the wave function. Then the state of our system is described by the state vector $|\psi(x, t)\rangle$ at any time. This state vector belongs to a Hilbert space. The evolution of the system is described by means of a wave function that satisfies the Schrödinger equation. This picture can be reformulated in fiber bundle terms (Asorey *et al.*, 1982).

Let $\xi(\pi, R^1, \mathscr{H})$ be the total fiber bundle space, where R^1 is a one-dimensional base space (or time axis), $\mathscr{H}$ is an infinite-dimensional Hilbert space or typical fiber, and $\pi: \xi \to R^1$ is the projection. In this "stationary" case all fibers are identical to each other; moreover, the frames of all typical fibers differ only by unitary transformations. The typical fiber frame is determined by the set of time-independent solutions of the stationary Schrödinger equation

$$\mathbf{H}|\psi(x, t)\rangle = E_n|\psi(x, t)\rangle$$

It is clear that the 1-form of connection in this fiber bundle is $\sigma(x) = i\mathbf{H}\, dt$ and the Schrödinger equation is the equation of parallel transport of the state vector from fiber $\mathscr{H}(t)$ to fiber $\mathscr{H}(t+dt)$. So

$$d|\psi(x, t)\rangle = -i\mathbf{H}\, dt|\psi(x, t)\rangle \tag{2.1}$$

The connection $i\mathbf{H}\, dt$ is an anti-Hermitian operator acting in $\xi(\pi, R^1, \mathscr{H})$. Note that the fiber bundle $\xi(\pi, R^1, \mathscr{H}) \cong R^1 \otimes \mathscr{H}$ is a trivial one in our case. The evolution operator $U(t_0, t_1) = \exp[(i/h)\mathbf{H}(t_1 - t_0)]$ defines the transport of the state vector along the path $t_0 \to t_1$ in R^1.

The operators of observables are governed by the Heisenberg equation

$$d\mathbf{F} + [i\mathbf{H}\, dt, d\mathbf{F}] = 0 \tag{2.2}$$

which can be treated as a parallel transport equation in the fiber bundle of operators $\xi(\pi, R^1, \mathfrak{F})$, where $\mathfrak{F}$ is the typical fiber or the set of Hermitian operators acting in $\xi(\pi, R^1, \mathfrak{F})$. These operators form the algebra of observables. Note that geometrical constructions on the operator fiber bundle (connection, curvature, etc.) are defined only by means of the Hamiltonian $\mathbf{H}$, so that this geometrical description is very simple. But the geometrical approach will be more far-reaching and useful in the consideration of systems with time-dependent Hamiltonians.

Let the Hamiltonian $\mathbf{H}(\mathbf{x}, \mathbf{p}, \alpha_i(t))$ be a function of slowly changing parameters $\{\alpha_i(t)\}$. Formally, here the function $\psi(x, t) = \langle x|\psi\rangle$ satisfies the Schrödinger equation $i\hbar\, \partial\psi/\partial t = \mathbf{H}\psi$. It is possible to form the Hilbert space at any time and it can be regarded as a fiber in some fiber bundle. Each fiber is assigned the frame $\{|n, \alpha_i(t)\rangle\}$. The frame is the set of eigenfunctions of the instantaneous Hamiltonian

$$\mathbf{H}(\mathbf{p}, \mathbf{x}; \alpha_i(t))|n, \alpha_i(t)\rangle = E_n(\alpha_i(t))|n, \alpha_i(t)\rangle \tag{2.3}$$

But the eigenfunctions belonging to different fibers (precisely, to different sheets of foliation) are not identical and are not connected by unitary transformations. We would like to underline that in the general case two fibers can be nonidentical to each other. To identify them we need to determine the special operator of mapping. We consider at this point only the usual case, when the fibers are identical but the frames of these fibers are different. This situation has been investigated in many papers (Asch, 1990; Berry, 1984; Buslaev, 1988; Hannay, 1985; Jackiw, 1988; Kiritsis, 1987; Montgomery, 1988; Simon, 1983). Note that in general the frames need not be eigenvectors of a specific operator. Namely, the frame is a more basic object than the parametrical Hamiltonian. According to the fiber bundle theory, we can construct $\xi(\pi, \mathcal{M}, \mathcal{H})$, where ξ is as usual the total fiber space, $\mathcal{M}$ is the base space for the parametrical manifold [its structure is defined by the set $\{\alpha_i(t)\}$], and $\mathcal{H}$ is the fiber or liner shell of eigenvectors. It is clear that frames belonging to different fibers cannot be transported by means of the above connection 1-form $i\mathbf{H}\, dt$ alone. To investigate an evolutionary picture for such a system, we need to determine a geometrical operator of parallel transport. This geometrical operator should be connected in some way with the connection 1-form

$$\Gamma_{mn} = \langle n|d|m\rangle \tag{2.4}$$

This connection was introduced by Simon (1983). But we think that the operator of eigenfunction transformations can be identical to the connection form (2.4) only in an infinitesimal neighborhood of any point of ξ. In the general situation we have to introduce a special operator mapping of the fibers. This operator should coincide with the connection locally but is not equivalent to Γ_{mn} globally. We should introduce the mapping operator from a quantum mechanical point of view but not from a geometrical one.

Let us mark the fibers by the letters $m, n, k, \ldots$. The mapping operator will be $\mathbb{P}(m, n)$ and it satisfies

(a) $\mathbb{P}|\psi_m\rangle = |\psi_n\rangle$

(b) $\mathbb{P}(\alpha|\psi_m\rangle + \beta|\psi_m\rangle) = \alpha\mathbb{P}|\psi_m\rangle + \beta\mathbb{P}|\psi_m\rangle, \quad \alpha, \beta \in \mathbb{C}$

(c) $\langle\psi_m|\mathbb{P}^+ = \langle\psi_n|$

(d) If $\mathbb{P}|\psi_m\rangle = |\psi_n\rangle$ and $\langle\psi_n|\psi_n\rangle = \langle\psi_m|\psi_n\rangle = 1$, then $\mathbb{P}^+\mathbb{P} = 1$

(e) $\mathbb{P}(m, n) = \mathbb{P}^{-1}(n, m)$

(f) $\mathbb{P}(m, m) = \mathbf{1}$ (2.5)

So we can write

$$|\psi_n\rangle = \mathbb{P}|\psi_m\rangle \cong (\mathbf{1} + \Gamma + \cdots)_{nm}|\psi_m\rangle \tag{2.6}$$

Now we use this mapping operator to investigate the evolution operator and Heisenberg equation.

2.2. Evolution Equation and Observables

Let us introduce the evolution operator as an operator which transports the state vector $|\psi(x, t)\rangle$ to the state vector $|\psi(x, t+\delta t\rangle$,

$$|\psi(x, t+\delta t\rangle = \mathbf{U}(t+\delta t, t)|\psi(x, t)\rangle \tag{2.7}$$

The evolution operator is not equal to the mapping operator, because the latter is a pure geometrical one and is not dependent on the Hamiltonian, but the evolution operator will be a functional of the Hamiltonian.

We can rewrite the Schrödinger equation as

$$i\hbar\, \nabla_t|\psi\rangle = \mathbf{H}(\mathbf{p}, \mathbf{x}; \alpha_i(t))|\psi\rangle \tag{2.8}$$

where

$$\nabla_t|\psi\rangle = \lim_{\delta t \to 0} \frac{\mathbb{P}(t, t+\delta t)|\psi(t+\delta t)\rangle - |\psi(t)\rangle}{\delta t} \tag{2.9}$$

Using (2.7), it is easy to obtain the equation for the operator $\Omega(t_1, t_2, t) = \mathbb{P}(t_1, t)U(t, t_2)$,

$$i\hbar \frac{\Omega(t_1, t_2, t)}{\partial t} = \mathbb{P}(t_1, t)\mathbf{H}(t)\mathbb{P}(t, t_2)\Omega(t_1, t_2, t) \tag{2.10}$$

Then

$$U(t_1, t_2) = T\exp\left\{-\frac{i}{h}\int_{t_1}^{t_2} \mathbb{P}(t_1, \tau)\mathbf{H}(\tau)\mathbb{P}(\tau, t_2)\, d\tau\right\} \tag{2.11}$$

If we decompose $\mathbb{P}(t_1, t)$ due to (2.6), then

$$\mathrm{U}(t_1, t_2) \cong T \exp\left\{-\frac{i}{h}\int_{t_1}^{t_2} \mathbf{H}(\tau)\, d\tau - \frac{i}{\hbar}\int_{t_1}^{t_2} [\mathbf{H}, \Gamma]\, d\tau + \cdots\right\} \tag{2.12}$$

Equation (2.12) takes the ordinary form if and only if $[\mathbf{H}, \Gamma] = 0$. It is true for any time-independent operator $\mathbf{H}$.

To get the equation for the operator $\mathbf{F}$ that corresponds to a dynamical variable, we need to take into account that $\mathbf{F}$ can be introduced by the set of its own eigenfunctions at any moment of time. So, we can introduce an operator fiber bundle, and we can consider that the geometrical structures of this bundle space are the same as in the above case. To consider the time derivative of $\mathbf{F}$ we use an equation analogous to (2.9). Then after very simple calculations we get

$$i\hbar \frac{d\mathbf{F}}{dt} = [\mathbf{F}, \mathbf{H}] + i\hbar \mathbf{U}^{-1}\left(\mathbb{P} \frac{\partial}{\partial t} (\mathbb{P}^{-1}\mathbf{F}\mathbb{P})\mathbb{P}^{-1}\right)\mathbf{U} \tag{2.13}$$

or in the local form

$$i\hbar \frac{d\mathbf{F}}{dt} \cong [\mathbf{F}, \mathbf{H}] + i\hbar \frac{\partial}{\partial t} [\mathbf{F}, \Gamma] + \cdots \tag{2.14}$$

This equation is different from the ordinary Heisenberg equation due to the second term. It is clear that this fact will lead to some change in the proof of Ehrenfest's theorem. We do not discuss the proof here but in the last section we will use equation (2.14).

3. TOPOLOGICAL NATURE OF BERRY'S PHASE

We mentioned in the Introduction that Berry found that the usual form of the quantum adiabatic theorem is not quite valid. He showed that an additional phase factor is acquired by the state vector. This new phase depends on the geometry of the parameter space. The observable values are the average ones from the operators with respect to new eigenvectors.

To investigate the topological nature of Berry's phase we consider here an arbitrary system of frame vectors in a fiber. Let $\mathbf{F}$ be an operator, and let $\{|f_n\rangle\}$ be the set of its eigenvectors in one of the fibers $\mathscr{H}(t)$. This operator does not determine the unique basis for $\mathscr{H}(\underset{\sim}{t})$, but it determines a set of bases which are different on unitary transformations $|f'_n(\underset{\sim}{t})\rangle \to \exp[i\rho(\underset{\sim}{t})]|f_n(\underset{\sim}{t})\rangle$, where the wavy underscore denotes the "instantaneous" fiber. Let us consider the value $\langle f_n|\nabla_t|f_n\rangle$. It is clear that for $|f'_n(t)\rangle = e^{i\rho(t)}|f_n(t)\rangle$

$$\langle f'_n|\nabla_t|f'_n\rangle - \langle f_n|\nabla_t|f_n\rangle = i\dot{\rho}(t) \neq 0 \tag{3.1}$$

If the eigenvectors form an orthogonal set, then $\langle f_n|\nabla_t|f_n\rangle$ is the pure imaginary value. The connection form can be introduced in the ordinary manner as

$$\Gamma_t^{mn} = \langle f_n|\nabla_t|f_m\rangle = \langle f_n| \lim_{\delta t\to 0} \frac{\mathbb{P}(t, t+\delta t)|f_m(t+\delta t)\rangle - |f_m\rangle}{\delta t} \tag{3.2}$$

and the Schrödinger equation in an arbitrary frame is

$$i\hbar \frac{\partial}{\partial t}(|f_n\rangle\langle f_n|\psi\rangle) = \mathbf{H}(|f_n\rangle\langle f_n|\psi\rangle) \tag{3.3}$$

We denote $a_n(t) = \langle f_n|\psi\rangle$; then, after multiplying (3.3) on $\langle f_n|$ and averaging we get the equation for $a_n(t)$,

$$\frac{\partial a_n}{\partial t} = -\Gamma^n_{tn} a_n - \Gamma^m_{tn} a_m - \langle f_n| \frac{i}{\hbar} \mathbf{H}|f_m\rangle a_m \tag{3.4}$$

This equation has a simpler form in the case $|f_n\rangle \equiv |E_n\rangle$, where $\mathbf{H}|E_n\rangle = E_n|E_n\rangle$; then

$$\langle E_n| \frac{i}{\hbar} \mathbf{H}|E_m\rangle a_m = \frac{i}{\hbar} E_n a_n \tag{3.5a}$$

and

$$\Gamma^m_{tn} = \frac{\langle E_m|\nabla_t|E_n\rangle}{E_m - E_n} \qquad \text{if} \quad n \neq m \tag{3.5b}$$

The adiabatic approximation is the condition of the "slow" variation of the parameters in the quantum system. This leads to a continuous transition of the system from one state to another at an infinite time period, and in an infinitely fast transition the system state does not change. From the geometrical point of view this is equivalent to the statement that $\Gamma^m_{tn} \cong 0$ for $n \neq m$ and $\Gamma^n_{tn} \neq 0$. Equation (3.4) has a solution in the adiabatic approximation, given by

$$a_n(t) = \exp\left\{-\frac{i}{\hbar}\int_0^t E_n(s)\, ds\right\} \exp(i\gamma_n) \tag{3.6}$$

where

$$\gamma_n = -i\int_0^t \Gamma^n_{tn}(s)\,ds = -i\int_0^t \langle E_n|\nabla_t|E_n\rangle\,ds \tag{3.7}$$

is a real value which is called "Berry's phase."

Now we can introduce the natural condition for removability of Berry's phase, namely

$$i\oint_c \Gamma^n_{tn}(s)\,ds = 2\pi n, \qquad n=0,1,2,\ldots \tag{3.8}$$

Due to the arbitrariness of the basis eigenfunctions, the condition (3.8) is a condition on the topology of the parameter manifold and of our fiber bundle. The topological classification of fiber bundles with Ehresmann connection can be performed (Kiritsis, 1987; Sadun and Segert, 1989). Our result (3.8) is the simplest demonstration of the fact that observable consequences of the nonholonomic structure of state space depend on the existence of closed geodesic curves on the parametrical manifold. Now we consider some physical applications of this approach.

4. HARMONIC OSCILLATOR, PARTICLE CREATION, AND BERRY'S CONNECTION

The investigation of quantum particle creation in external fields (Ivanenko and Sokolov, 1955; Parker, 1968; Zeldovich and Starobinsky, 1971) leads to the problem of the parametric excitation of an oscillator (Grib *et al.*, 1980). The problems of particle interpretation and vacuum concept have been discussed by a number of authors and are given fully by Grib *et al.* (1980). We discuss here only the connection between this effect and Bogolubov's transformations in the light of the geometrical approach to quantum mechanics and the nonholonomic phase.

4.1. Matrix Representation

The Hamiltonian of an oscillator with a time-dependent frequency is

$$\mathbf{H}(t) = \frac{\mathbf{p}^2}{2M} + \frac{M\omega^2(t)}{2}\mathbf{x}^2 \tag{4.1}$$

Let us introduce creation and annihilation operators for the instantaneous Hamiltonian

$$\mathbf{a} = \frac{1}{\sqrt{2}}\left(\zeta + \frac{\partial}{\partial\zeta}\right), \qquad \mathbf{a}^+ = \frac{1}{\sqrt{2}}\left(\zeta - \frac{\partial}{\partial\zeta}\right) \tag{4.2}$$

where $\zeta = x/x_0$ and $x_0(\hbar/M\omega^2)^{1/2}$.

These operators satisfy the commutator relations

$$[\mathbf{a}, \mathbf{a}] = [\mathbf{a}^+, \mathbf{a}^+] = 0, \qquad [\mathbf{a}, \mathbf{a}^+] = \mathbb{1}$$

The instantaneous Hamiltonian in terms of $\mathbf{a}$ and $\mathbf{a}^+$ is

$$\mathbf{H} = \hbar\omega(t)(\mathbf{a}^+\mathbf{a} + \mathbf{a}\mathbf{a}^+) \tag{4.3}$$

At any moment of time we can find the orthogonal set of eigenfunctions

$$\mathbf{H}|E_n, t\rangle = E_n(t)|E_n, t\rangle \tag{4.4a}$$

where

$$|E_n, t\rangle = \frac{1}{(2^n n! \sqrt{\pi}\, x_0)^{1/2}} e^{-\zeta^2/2} H_n(\zeta) \tag{4.4b}$$

and $H_n(\zeta)$ are Hermite polynomials, which satisfy the usual algebraic-differential relations

$$\begin{aligned} H_n(\zeta) &= (-1)^n e^{\zeta^2} d^n e^{-\zeta^2}/d\zeta^n \\ H_{n+1}(\zeta) &= 2\zeta H_n(\zeta) - 2n H_{n-1}(\zeta) \\ dH_n(\zeta)/d\zeta &= 2n H_{n-1}(\zeta) \\ E_n(t) &= \hbar\omega(t)(n + \tfrac{1}{2}) \end{aligned} \tag{4.5}$$

From the geometrical point of view it is possible to define two fiber bundles, the state fiber bundle with fiber $\{|E_n, t\rangle\}$ and the operator fiber bundle with the fiber $\{\mathbf{a}, \mathbf{a}^+, \ldots\}$. The creation and annihilation operators act in any fiber as

$$\begin{aligned} \mathbf{a}|E_n, t\rangle &= n^{1/2}|E_{n-1}, t\rangle \\ \mathbf{a}^+|E_n, t\rangle &= (n+1)^{1/2}|E_{n+1}, t\rangle \end{aligned} \tag{4.6}$$

The wave function is a section of the fiber bundle. Then in accordance with the ideology of Section 2 we represent

$$|\psi(x, t)\rangle = \sum_n C_n(t)|E_n, t\rangle$$

Then $\Gamma^m_{tn} = \langle E_n, t|(d/dt)|E_m, t\rangle$, and it is easy to verify that only

$$\Gamma^{n-2}_{tn} = \frac{\dot{\omega}}{2\omega}[n(n-1)]^{1/2}, \qquad \Gamma^{n+2}_{tn} = -\frac{\dot{\omega}}{2\omega}[(n+2)(n+1)]^{1/2} \tag{4.7}$$

are not equal to zero. So, the nonholonomic phase effect is absent at this stage.

Now let us write down the equations for $\{C_n(t)\}$, which are consequences of (3.4):

$$
\begin{aligned}
\dot{C}_0(t)+\frac{i}{\hbar}E_0(t)C_0(t)&=\frac{\dot{\omega}}{2\omega}2^{1/2}C_2(t)\\
\dot{C}_1(t)+\frac{i}{\hbar}E_1(t)C_1(t)&=\frac{\dot{\omega}}{2\omega}6^{1/2}C_3(t)\\
&\vdots\\
\dot{C}_{2n}(t)+\frac{i}{\hbar}E_{2n}(t)C_{2n}(t)&=\frac{\dot{\omega}}{2\omega}\{-[2n(2n-1)]^{1/2}C_{2(n-1)}(t)\\
&\quad+[(2n+1)(2n+2)]^{1/2}C_{2(n+1)}(t)\}\\
\dot{C}_{2n+1}(t)+\frac{i}{\hbar}E_{2n+1}(t)C_{2n+1}(t)&=\frac{\dot{\omega}}{2\omega}\{-[2n(2n+1)]^{1/2}C_{2n+1}(t)\\
&\quad+[(2n+2)(2n+3)]^{1/2}C_{2n+3}(t)\}
\end{aligned}
\tag{4.8}
$$

This system can be represented in the compact matrix form

$$
i\hbar\frac{\partial\mathbb{C}}{\partial t}=(\mathbf{H}+i\hbar\Gamma)\mathbb{C} \tag{4.9}
$$

where $\mathbb{C}$ is a column vector and $\mathbf{H}$ and Γ are matrices,

$$
\mathbb{C}=\begin{bmatrix} C_0\\ C_1\\ \vdots\\ C_n\\ \vdots \end{bmatrix},\qquad
\mathbf{H}=\begin{bmatrix}
E_0 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\\
0 & E_1 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot\\
0 & 0 & E_2 & 0 & 0 & \cdot & \cdot & \cdot & \cdot\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
0 & \cdot & \cdot & \cdot & \cdot & \cdot & E_n & 0 & \cdot\\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{bmatrix}
$$

$$
\Gamma=\frac{\dot{\omega}}{2\omega}\begin{bmatrix}
0 & 0 & \sqrt{2} & 0 & 0 & \cdot & \cdot & \cdot\\
0 & 0 & 0 & 0 & \sqrt{6} & \cdot & \cdot & \cdot\\
-\sqrt{2} & 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot\\
0 & 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot\\
0 & -\sqrt{6} & 0 & 0 & \cdot & \cdot & \cdot & \cdot\\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
\end{bmatrix} \tag{4.10}
$$

So the Schrödinger equation can be represented in matrix (or energy) form. In contrast to the time-independent Hamiltonian, the column function satisfies an equation with an effective Hamiltonian $\mathbf{H}_{\text{eff}}=\mathbf{H}+i\hbar\Gamma$. The formal solution of (4.9) is

$$\mathbb{C}=\exp\left\{-\frac{i}{\hbar}\int(\mathbf{H}+i\hbar\Gamma)\,ds\right\}\cdot\mathbb{C}_0 \tag{4.11}$$

The last expression can be rewritten in the form

$$\mathbb{C}=\exp\left\{-\frac{i}{\hbar}\int\mathbf{H}\,ds\right\}\exp\left\{\int\Gamma\,ds\right\}\cdot\mathbb{C}_0 \tag{4.12}$$

if and only if $[\mathbf{H},\Gamma]=0$. But it is not valid in every situation. If the commutator of two operators is equal to zero, this means that these operators have a common set of eigenfunctions. But it is obvious that eigenfunctions of $\mathbf{H}$,

$$|0\rangle=\begin{bmatrix}1\\0\\0\\0\\\vdots\end{bmatrix},\qquad |1\rangle=\begin{bmatrix}0\\1\\0\\0\\\vdots\end{bmatrix},\qquad \text{etc.}$$

will not be eigenfunctions of Γ. This indicates that one needs to take into consideration the contributions of $\langle\Gamma\rangle$ in some situations. We can neglect these contributions only by a specific choice of state bundle. To show that in some situations the nonholonomic contributions can be considerable, we consider the coordinate form of Γ.

4.2. Coordinate Representation of Γ

We denote the eigenfunctions of the effective Hamiltonian $\mathbf{H}_{\text{eff}}=\mathbf{H}+i\hbar\Gamma$ as $|\tilde{n},t\rangle$. These functions are column matrices and are governed by the equation

$$(\mathbf{H}+i\hbar\Gamma)|\tilde{n},t\rangle=E_{\tilde{n}}|\tilde{n},t\rangle \tag{4.13}$$

The new basis $\{|\tilde{n},t\rangle\}$ is not equivalent to the old one $\{|n,t\rangle\}$, $\mathbf{H}|n,t\rangle=E_n|n,t\rangle$, and it is clear now that $\langle n,t\rangle|\nabla_t|n,t\rangle=0$, but $\langle\tilde{n},t|\nabla_t|\tilde{n},t\rangle\neq0$. The effective Hamiltonian gives the new spectrum (set of energy levels). Let us consider the connection of two spectra $\{E_n\}$ and $\{E_{\tilde{n}}\}$. Taking into account (4.13), we get

$$\langle n,t|\mathbf{H}_{\text{eff}}|\tilde{n},t\rangle=\langle n,t|\mathbf{H}_{\text{eff}}|m,t\rangle\langle m,t|\tilde{n},t\rangle$$

Then

$$\langle n, t|E_{\tilde{n}}|\tilde{n}, t\rangle = i\hbar\langle n, t|\Gamma|m, t\rangle\langle m, t|\tilde{n}, t\rangle$$

In the adiabatic approximation

$$i\hbar\Gamma^{n}_{tn} = i\hbar\langle n, t|\Gamma|n, t\rangle = E_{\tilde{n}} - E_n \tag{4.14}$$

Here $n = \tilde{n}$, but the tilde is needed to underline the fact that $E_{\tilde{n}}$ and E_n belong to different spectra.

Now it is clear that the nonholonomic phase has a nonlocal nature, because it is a function of different spectra. In the general case the discrepancy $E_{\tilde{n}} - E_n$ is not a unique-valued function and we can make it equal to zero.

Starting from (3.2) and (4.14), we determine the coordinate representation of the connection operator as

$$\Gamma = \frac{i\dot{\omega}}{2\hbar\omega}(\mathbf{xp} + \mathbf{px}), \qquad \mathbf{p} = -i\hbar\frac{\partial}{\partial x} \tag{4.15}$$

It is easy to verify that $\langle n, t|\Gamma|n, t\rangle$ coincides with (4.13), (4.14) if we take into consideration the properties of the Hermite polynomials (4.5). The initial problem now can be regarded as a new dynamical system which is described by the effective Hamiltonian

$$\mathbf{H}_{\text{eff}} = \frac{\mathbf{p}^2}{2M} + \frac{M\omega^2}{2}\mathbf{x}^2 - \frac{\dot{\omega}}{2\psi}(\mathbf{xp} + \mathbf{px}) \tag{4.16}$$

Note that this representation was found due to the special choice of the basis in fiber. Let us consider now properties such as the transformations $\{|n, t\rangle\} \to \{|\tilde{n}, t\rangle\}$ in the light of the appearance and removal of Berry's phase and particle creation.

4.3. Canonical Transformations and Diagonalization of Hamiltonian

The Hamiltonian (4.16) belongs to a well-investigated class of Hamiltonians and it is well known that Berry's phase is not equal to zero for such systems (Jackiw, 1988). The connection operator Γ can be rewritten in terms of creation and annihilation operators (4.2) and is

$$\Gamma = \frac{\dot{\omega}}{2\omega}(\mathbf{aa} - \mathbf{a}^+\mathbf{a}^+) \tag{4.17}$$

So the effective Hamiltonian takes the form

$$\mathbf{H}_{\text{eff}} = \hbar\omega(t)(\mathbf{a}^+\mathbf{aaa}^+) + i\hbar\frac{\dot{\omega}}{2\omega}(\mathbf{aaa}^+\mathbf{a}^+) \tag{4.18}$$

The diagonalization of (4.18) can be made due to Bogolubov's transformations

$$\begin{aligned} \mathbf{b} &= \Phi^*\mathbf{a} - \Psi\mathbf{a}^+ \\ \mathbf{b}^+ &= \Phi\mathbf{a}^+ - \Psi^*\mathbf{a} \end{aligned} \tag{4.19}$$

where $\Phi(t)$ and $\Psi(t)$ are complex functions and $|\Phi|^2 - |\Psi|^2 = 1$.

Let us require the diagonal form of $\mathbf{H}_{\text{eff}}$ in terms of new operators, namely

$$\mathbf{H}_{\text{eff}} = A\mathbf{b}^+\mathbf{b} + D \tag{4.20}$$

Then after some algebra we find

$$\mathbf{H}_{\text{eff}} = \hbar\omega\,\frac{1-4\gamma^2}{2}\,\mathbf{b}^+\mathbf{b} + \frac{\hbar\omega}{2}\left\{1 + \frac{1}{\sqrt{2}}[1-(1-4\gamma^2)^{1/2}]\right\} \tag{4.21}$$

where $\gamma = \dot{\omega}/2\omega^2$.

The Hamiltonian (4.21) is the same as the initial Hamiltonian, but with a different frequency and vacuum energy level. It is clear that from the geometrical point of view this arbitrariness is deeply connected with the choice of the holonomic basis in the fiber. Finally we would like to underline that the holonomic frames are the eigenfunctions of the diagonal Hamiltonians, but the nonholonomic frames are the eigenfunctions of the nondiagonal Hamiltonians. We think that this fact has important physical significance since the problem of particle creation is based on a consideration of a procedure of Hamiltonian diagonalization.

5. PARTICLE IN A WELL WITH MOVING WALL

As an example of a dynamical system with nonstationary boundary conditions let us consider a particle in a potential well with a moving wall, the potential being

$$V(x) = \begin{cases} 0, & x \in [0, L(t)] \\ \infty, & \text{otherwise} \end{cases} \tag{5.1}$$

Then the Hamiltonian of the particle inside this well takes the form

$$\mathbf{H}_0 = \frac{\mathbf{p}^2}{2M} \tag{5.2}$$

The quantum state of the particle is described by the wave function governed by the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \mathbf{H}_0 \psi(x, t) \tag{5.3}$$

endowed with boundary conditions

$$\psi(x=0, t) = 0 = \psi(x = L(t), t) \tag{5.4}$$

The wave function $\psi(x, t)$ can be decomposed into the sum

$$\psi(x, t) = \sum_n a_n(t) |\psi_n(x, t)\rangle$$

where $|\psi_n(x, t)\rangle$ are eigenfunctions of any operators, for example, we can take $\mathbf{H}_n |\psi_n(x, t)\rangle = E_n |\psi_n(x, t)\rangle$. Let us consider the action of the $\partial/\partial t$ operator on $|\psi_n(x, t)\rangle$. The usual definition

$$\frac{\partial |\psi_n(x, t)\rangle}{\partial t} = \lim_{\delta t \to 0} \frac{|\psi_n(x, t+\delta t)\rangle - |\psi_n(x, t)\rangle}{\delta t}$$

makes no sense because $|\psi_n(x, t+\delta t)\rangle$ and $|\psi_n(x, t)\rangle$ belong to different $\mathscr{L}^{(2)}_{[0,L(t)]}$ spaces. To determine correctly the action of the operator $\partial/\partial t$ it is necessary to map one $\mathscr{L}^{(2)}_{[0,L(t+\delta t)]}$ on another $\mathscr{L}^{(2)}_{[0,L(t)]}$. This mapping needs to satisfy the standard properties—to be smooth, conserve the boundary conditions, and the norm of the wave function. So we are to find a representation of the mapping operator $\mathbb{P}(t_1, t_2)$ such that

$$\mathbb{P}: \quad [0, L(t_1)] \Rightarrow [0, L(t_2)] \tag{5.5a}$$

and

$$\mathbb{P}: \quad \{|\psi_n(x, t_1)\rangle \in \mathscr{L}^{(2)}_{[0,L(t_1)]}\} \Rightarrow \{|\psi_n(x, t_2)\rangle \in \mathscr{L}^{(2)}_{[0,L(t_2)]}\} \tag{5.5b}$$

Because $[0, L(t)]$ is parametrized by coordinates $\mathbf{x}$, the action of $\mathbb{P}$ in coordinate representation is

$$\mathbb{P}: \quad \mathbf{x} \to \mathbf{x}' = \mathbf{x}\frac{L(t_1)}{L(t_2)}$$

Then a direct calculation leads to the simple infinitesimal form of $\mathbb{P}$ acting on $\{|\psi_n(x, t)\rangle\}$, namely

$$\mathbb{P} \cong 1 + \delta t \frac{\dot{L}}{2L}\left(x\frac{\partial}{\partial x} + \frac{\partial}{\partial x} x\right) \tag{5.6}$$

Now we can determine the correct form of the time derivative

$$\nabla_t|\psi_n(x, t)\rangle = \left\{\frac{\partial}{\partial t} + \frac{\dot{L}}{2L}\left(x\frac{\partial}{\partial x} + \frac{\partial}{\partial x}x\right)\right\}|\psi_n(x, t)\rangle \tag{5.7}$$

The Schrödinger equation has the form

$$i\hbar\,\nabla_t|\psi(x, t)\rangle = \mathbf{H}_0|\psi(x, t)\rangle$$

or, in a more usual form,

$$i\hbar\frac{\partial}{\partial t}|\psi(x, t)\rangle = \left\{\frac{\mathbf{p}^2}{2M} + \frac{\dot{L}}{2L}(\mathbf{xp} + \mathbf{px})\right\}|\psi(x, t)\rangle \tag{5.8}$$

Here we have introduced $\mathbf{p} = -i\hbar\,\partial/\partial x$.

Equation (5.8) is an improved form of the original one, because the time derivative is correctly defined.

We can consider the right-hand side of (5.8) as a new effective Hamiltonian operator acting on the wave function. The new Hamiltonian is equivalent to the Hamiltonian for a charged particle interacting with an electromagnetic field due to the "vector" potential

$$\mathscr{A}(x, t) = -\frac{Mc\dot{L}}{QL}x$$

In this case

$$\mathbf{H}_{\text{eff}} = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + \frac{Q\hbar}{Mc}i\left(\mathscr{A}\frac{\partial}{\partial x} + \frac{1}{2}\frac{\partial\mathscr{A}}{\partial x}\right) \tag{5.9}$$

So in a quantum system with a time-dependent boundary condition, the gauge field appears as a functional of the relative velocity of the well height changing in the adiabatic approximation.

To calculate the eigenfunctions and eigenvalues of the effective Hamiltonian we consider the additional term $(\dot{L}/2L)(\mathbf{xp} + \mathbf{px})$ as a small perturbation for the movement of a free particle inside the well. Then in the frame of ordinary perturbation theory the eigenfunctions and eigenvalues are

$$\begin{aligned} |\psi_n(x, t)\rangle &= |\psi_n^{(0)}(x, t)\rangle + |\psi_n^{(1)}(x, t)\rangle + \cdots \\ E_n &= E_n^{(0)} + E_n^{(1)} + \cdots \end{aligned} \tag{5.10}$$

where

$$|\psi_n^{(0)}(x,t)\rangle = \left[\frac{2}{L(t)}\right]^{1/2} \sin\left[\frac{\pi n x}{L(t)}\right]$$
$$E_n^{(0)} = \frac{\hbar^2\pi^2 n^2}{2ML(t)^2}, \qquad n\in\mathbb{Z} \tag{5.11}$$

After some uncomplicated calculations we get

$$|\psi_n^{(1)}(x,t)\rangle = \left(\frac{2}{L}\right)^{1/2}\left[\sin\left(\frac{\pi n x}{L}\right) - i\frac{4M\dot{L}\sqrt{L}}{\pi^2\hbar}\sum_k \frac{kn}{(k^2-n^2)^2}(-1)^{k+n}\sin\left(\frac{\pi n x}{L}\right)\right]$$
$$E_n^{(1)} = \frac{8M\dot{L}^2}{\pi^2}\sum_k \frac{k^2n^2}{(k^2-n^2)^3}, \qquad k\neq n$$

Now we can find the standard Berry phase and Berry connection

$$\Gamma_{tn}^n = \langle\psi_n|\frac{\partial}{\partial t}|\psi_n\rangle$$

The exact form of this connection is very complicated and we write here only the first term,

$$\Gamma_{tn}^n \cong 2\frac{M}{n^2}\frac{\dot{L}^2}{\hbar}$$

The Berry phase is

$$\gamma_n = i\int \Gamma\, dt \cong \frac{16M}{\hbar n^2\pi^2}\int_{L_0}^{L} \dot{L}\, dL$$

So we can see that time-dependent boundary conditions lead to the appearance of the Berry phase and the shift of energy levels $\Delta E_n \cong M\dot{L}^2/n^2$. Using equation (2.14), we find $\langle\partial \mathbf{x}/\partial t\rangle = \dot{L}/2$.

6. CONCLUSIONS

We have considered here the nonholonomic properties of dynamical systems with time-dependent Hamiltonian and boundary conditions. Using fiber bundle concepts makes it possible to study the evolution problem in a geometrical way. We showed that the Heisenberg equations should be supplemented by new geometrical type terms.

We conclude that the removability of Berry's phase due to the diagonalization of the Hamiltonian leads to an energy level shift and can be observed as a dynamical effect.

Moreover, we remark that the geometrical description can be extended to systems with nonstationary boundary conditions. The corresponding Berry phase was calculated, and the energy level shift was found.

In the work of Doescher and Rice (1969) the problem of a particle in a one-dimensional infinite square-well potential was considered when the velocity of the moving wall is constant. The exact solution of the Schrödinger equation (5.3) with time-dependent boundary conditions was obtained.

The recent work of Pinder (1990) was devoted to the extension of the method proposed first by Doescher and Rice (1969) for the case when the wall velocity is not constant. The author used perturbation theory. But we think that this is not the only method to solve the problem. Moreover, we consider that the application of perturbation theory in this case can lead to ambiguities, because a good mathematical description is constructed for the Hamiltonians $\mathbf{H}_1 = \mathbf{H}_0 + \varepsilon \mathbf{V}(x, t)$ when the eigenfunctions of $\mathbf{H}_1$ become the eigenfunctions of $\mathbf{H}_0$ in the limit $\varepsilon \to 0$. At the same time, a small change of boundary conditions can lead to an essential change of the initial eigenfunctions. That is why we reformulated the problem through the effective Hamiltonian. This gives us grounds for using perturbation theory and calculating the nonholonomic effects.

In another approach (Greenberger, 1988) the extra phase was derived by changing coordinates. We think that these two results (Greenberger's and ours) are two aspects of the same problem. But in Greenberger's work the so-called "phase factor" depends on both time and coordinates, so in our opinion it cannot be called a true "extra geometrical phase factor," since it is only part of the wave function. In our treatment the extra phase is the true "topological phase" obtained in Berry's spirit, and can be connected with the appearance of the additional gauge structure.

We believe that the use of geometrical conceptions for quantum systems with varying parameters will be a powerful tool, especially in the investigation of quantum measurement problems. We intend to discuss these problems in a forthcoming paper.

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