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Non-adiabatic quantum evolution: The S matrix as a geometrical phase factor

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This work is dedicated to the memory of Mr. A.L. Ayadi, head of the Agronomy Department, University Ferhat Abbas of Sétif, Algeria

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ABSTRACT

We present a complete derivation of the exact evolution of quantum mechanics for the case when the underlying spectrum is continuous. We base our discussion on the use of the Weyl eigendifferentials. We show that a quantum system being in an eigenstate of an invariant will remain in the subspace generated by the eigenstates of the invariant, thereby acquiring a generalized non-adiabatic or Aharonov–Anandan geometric phase linked to the diagonal element of the S matrix. The modified Pöschl–Teller potential and the time-dependent linear potential are worked out as illustrations.

1. Introduction

Quantum geometric phase have been attracting significant research interest in the recent 30 years. Berry [1] showed that, an eigenstate of parameter-dependent Hamiltonian $H(\vec{X}(t))$ varying adiabatically and cyclically acquires, besides the well-known dynamical phase $e^{-i\hbar^{-1}\int E_n(t)\,dt}$, a geometrical phase

$$\gamma_n^G(C) = \oint_C \langle \psi_n(\vec{X}) | i\hbar \vec{\nabla}_{\vec{X}} | \psi_n(\vec{X}) \rangle \, d\vec{X}, \tag{1}$$

which depends essentially on the closed path C that has been followed in the parameters space. As explained by Simon [2], the geometrical transport, along C, that brings an initial eigenstate to the evolved state, can be derived from the natural connection of the line bundle. Later, the geometric phase was, generalized to the cases of degenerate energy eigenstates by Wilczek and Zee [3].

Removing the adiabatic hypothesis, Aharonov and Anandan [4] have reformulated and generalized Berry's result and shown that such a geometrical phase may appear for any state which is cyclic with respect to some evolution. They defined their non-adiabatic geometrical phase for the cyclic evolution in the projective Hilbert space by removing the dynamical part, identified as the integral of the expectation value of the Hamiltonian $\hbar^{-1}\int_0^T \langle \Psi(t)|H(t)|\Psi(t)\rangle$, from the total phase φ. They showed that the geometrical phase can be written in the form

$$\beta^G = \int_0^T \langle \tilde{\psi}(t) | i\frac{d}{dt} | \tilde{\psi}(t) \rangle \, dt, \tag{2}$$

where $|\tilde{\psi}(t)\rangle = e^{-if(t)}|\Psi(t)\rangle$ with $f(T) - f(0) = \varphi$ such that $|\tilde{\psi}(T)\rangle = |\tilde{\psi}(0)\rangle$. The cyclic states can be obtained as eigenstates of a periodic invariant operator $I(T) = I(0)$ introduced by Lewis and Riesenfeld [5]. In general, even for non-adiabatic, non-unitary and non-cyclic evolutions, a reparametrization invariant phase can be defined which is associated with a curve in the ray space [6,7].

In their classical paper on dynamical invariant $I(t)$, Lewis and Riesenfeld [5] are very close to discover the geometric phase. They showed that for a quantal system characterized by a time-dependent Hamiltonian $H(t)$ and a Hermitian invariant operator $I(t)$, the eigenstate $|\phi_n(t)\rangle$ of $I(t)$ develops a global phase given by

$$\hbar\theta_n(t) = \int_0^t \langle \phi_n(t') | \left[i\hbar \frac{\partial}{\partial t'} - H \right] | \phi_n(t') \rangle \, dt', \tag{3}$$

where

$$\hbar\theta_n^g(t) = \int_0^t \langle \phi_n(t') | i\hbar \frac{\partial}{\partial t'} | \phi_n(t') \rangle \, dt', \tag{4}$$

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has been interpreted as a non-adiabatic geometrical phase after Berry's phase discovery. The correspondence of Berry's phase and Lewis–Riesenfeld phase has been pointed out by Morales [8] for the case of quadratic Hamiltonians. Notice that Berry's analysis corresponds to the case where $H(0) = I(0)$ (and an adiabatic evolution) and the one of Aharonov–Anandan to the case $I(0) = |\tilde{\psi}(0)\rangle\langle\tilde{\psi}(0)|$ (and a cyclic evolution).

Most of the works on both geometrical phase and the invariant theory are confined to discrete spectra. In the case of continuous spectra, such as in the scattering theory, Newton [9] within non-interaction picture method revealed that its geometric phase factor is connected to the S matrix. In order to reinterpret the usual scattering phase shift as an adiabatic phase in the spirit of the original investigation of Berry, Ghosh [10] extended the adiabatic approximation to the continuous spectra like an *ansatz* and confined the derivation to a one-dimensional scattering problem with negligible reflection.

Using the Weyl eigendifferentials [12,13]

$$\left|\delta\phi_k(t)\right\rangle = \int_k^{k+\delta k} \left|\phi_{k'}(t)\right\rangle dk' \tag{5}$$

which in some sense "technically discretizes" the continuous spectrum and lays the basis for transferring all the concepts known for discrete spectra to the continuous case, Maamache and Saadi [11] have proved the adiabatic theorem for Hamiltonian systems with continuous spectra and addressed the corresponding generalization of the concept of the adiabatic Berry's phase to the continuous case

$$\gamma_k^G(t) = \int_0^t \left\langle\delta\psi_k\left(t'\right)\right|i\hbar\frac{\partial}{\partial t'}\left|\psi_k\left(t'\right)\right\rangle dt' \tag{6}$$

($|\psi_k(t)\rangle$ is an eigenstate of the instantaneous Hamiltonian) and showed that the generalized geometrical phase is the diagonal element of the S matrix, yielding a consistent picture. Very recently, Liu and Yi [14] explored the geometric phase in the scattering process by taking only the transmission process into account.

Important questions motivate our work: How could one treat the time-dependent quantum problems for a continuous spectrum and investigate the possibility of finding geometric phases related to the invariant operator theory? Should the S matrix conserve its geometric aspect without recourse to adiabaticity (i.e. in a cyclic evolution)? The key idea in this Letter is the use of the Weyl eigendifferentials in order to present a theoretical proof of the exact quantum evolution for systems whose Hamiltonians and their invariants have a completely continuous spectrum supposed to be non-degenerated. The expression for the obtained total phase is expressed in terms of the eigenvectors of the invariant operator. Once the generalization of the invariants theory is established, we show, based on the cyclicity of the scattering problems, that the geometric aspect of the S matrix is independent of the nature of the time evolution of the system.

2. Exact evolution for continuous spectrum

2.1. Review of the discrete spectrum case

Let us recall that the general method to introduce the Lewis and Riesenfeld theory, valid whatever the time dependence of the parameters, considers invariant operators. For a system specified by a time-dependent Hamiltonian $H(t)$, and a corresponding evolution operator $U(t)$, an invariant is an operator $I(t)$ such that

$$\frac{dI}{dt} = \frac{\partial I}{\partial t} + \frac{1}{i\hbar}[I, H] = 0. \tag{7}$$

We note that in view of Eq. (7) any dynamical invariant satisfies

$$I(t) = U(t)I(0)U^{-1}(t). \tag{8}$$

It possesses a remarkable property that any eigenstate $|\phi_n(0)\rangle$ of an invariant operator at time zero $I(0)$ evolves continuously into the corresponding eigenstate $|\phi_n(t)\rangle$ of the invariant operator $I(t)$ at time t (each eigenstate is associated with the time-independent eigenvalue λ_n),

$$\left|\Psi_n(t)\right\rangle = U(t)\left|\phi_n(0)\right\rangle = e^{i\theta_n(t)}\left|\phi_n(t)\right\rangle \tag{9}$$

exactly as an eigenstate of the Hamiltonian does when the evolution is adiabatic. It follows from the Schrödinger equation $(i\hbar\partial/\partial t - H(t))|\Psi_n(t)\rangle = 0$ that the corresponding global phase $\theta_n(t)$ satisfies the relation (3).

One way to describe the Lewis and Riesenfeld's exact quantum evolution is to introduce the concept of elementary projectors on an eigenstate $|\phi_n(t)\rangle$ of the invariant operator $I(t)$

$$P_n(t) = \left|\phi_n(t)\right\rangle\left\langle\phi_n(t)\right|. \tag{10}$$

It is easy to verify that each projector $P_n(t)$ is therefore a constant of motion, i.e., $P_n(t) = U(t)P_n(0)U^+(t)$, and the exact evolution can be formally written, in terms of the evolution operator as

$$\forall t: \quad U(t)P_n(0) = P_n(t)U(t). \tag{11}$$

Notice that if, initially, the system is in the eigenstate $|\phi_n(0)\rangle$ so that $I(0)|\phi_n(0)\rangle = \lambda_n|\phi_n(0)\rangle$, then

$$P_n(0)\left|\phi_n(0)\right\rangle = \left|\phi_n(0)\right\rangle \tag{12}$$

and (11) gives

$$U(t)\left|\phi_n(0)\right\rangle = P_n(t)U(t)\left|\phi_n(0)\right\rangle. \tag{13}$$

2.2. Generalization to the continuous spectrum case

The Lewis and Riesenfeld theory in a continuous spectrum was raised for the first time by Hartley and Ray [15] where they extended this theory for a general Ermakov system to cases where the invariant has continuous eigenvalues. They looked, as an *ansatz*, at the eigenfunctions in a continuous spectrum $|\phi_k(t)\rangle$ of the invariant operator $I(t)$ and the solution $|\Psi_k(t)\rangle$ of the Schrödinger equation in the form

$$\left|\Psi_k(t)\right\rangle = e^{i\theta_k(t)}\left|\phi_k(t)\right\rangle. \tag{14}$$

The limitation of the Hartley–Ray approach is that, in general, there is no explicit formula of Lewis and Riesenfeld phase and they didn't deal with problems having continuous spectra of origin. In the following, we will show that (14) is a solution of the Schrödinger equation, this has not been shown before in the continuous case.

To find the phase, usually most authors [16] will substitute the solution (14) into the Schrödinger equation which leads to the following result

$$\hbar\frac{d}{dt}\theta_k(t)\left|\phi_k(t)\right\rangle = \left[i\hbar\frac{\partial}{\partial t} - H\right]\left|\phi_k(t)\right\rangle, \tag{15}$$

and then project this equation onto the $\langle\phi_k(t)|$ (this procedure is clearly parallel to that for the discrete case), it follows that the corresponding global phase $\theta_k(t)$ satisfies the relation $\hbar\frac{d}{dt}\theta_k(t)\delta(0) = \langle\phi_k(t)|[i\hbar\frac{\partial}{\partial t} - H]|\phi_k(t)\rangle$ which is infinite, i.e., $\delta(0) = \infty$. In fact, it's well known and easily shown that the term $\langle\phi_k(t)|[i\hbar\frac{\partial}{\partial t} - H]|\phi_{k'}(t)\rangle$ is a one-point support distribution,