Adiabatic Theorem and Generalized Geometrical Phase in the Case of Continuous Spectra

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By defining "*a virtual gap*" for the continuous spectrum through the notion of eigendifferential (Weyl's packet) and using the differential projector operator, we present a rigorous demonstration and discussion of the quantum adiabatic theorem for systems having a nondegenerate continuous spectrum. An explicit formula for a generalized geometrical phase is derived in terms of the eigenstates of the Hamiltonian. Examples are given for illustration.

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The adiabatic theorem (AT) is one of the basic results in quantum theory [1]. It is concerned with quantum systems described by an explicitly, but slowly, time-dependent Hamiltonian. This AT concerns states $|\psi(t)\rangle$ satisfying the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \tag{1}$$

and asserts that if a quantum system with a time-dependent nondegenerate Hamiltonian $H(t)$ is initially in the nth eigenstates of $H(0)$, and if $H(t)$ evolves slowly enough, then the state at time t will remain in the nth instantaneous eigenstates of $H(t)$ up to a multiplicative phase factor $\phi_n(t)$. There has been a sudden regain of interest in the AT for itself among physicists when in 1984, M. V. Berry [2] pointed out that if it was applied to Hamiltonians, whose parameters vary slowly in time and has been confined to discrete spectrum, satisfying $H(t_1) = H(t_2)$, it could generate a geometrical phase (GP) factor $e^{\gamma_n^B}$. This is a part from the familiar dynamical phase factor $e^{-(i/\hbar)\int E_n(t)dt}$ associated with the time evolution of the state being so transported with instantaneous eigenenergy $E_n(t)$, depending only on the curve C which has been followed in the parameters space. And more recently, the AT has renewed its importance in the context of quantum control [3], for example, concerning adiabatic passage between atomic energy levels, as well as for adiabatic quantum computation [4].

There are several points of view for a discussion of the quantum AT [5–7]; each one offers interesting insight. Let us simply recall here that works [1,5,6] have led to a formulation of the AT under the usual gap assumption $g_{nm}(t) = E_n(t) - E_m(t)$, between level n and m. One may then state that a general validity condition for adiabatic behavior is well controlled as follows: the larger is the quantity $\min_{0\le t\le T,m}|g_{nm}(t)|$, the smaller will be the transition probability.

Despite the existence of extensive literature on rigorous proofs of estimates needed to justify the adiabatic approximation (AA) [1,6–8], doubts have been raised about its validity [9] leading to confusion about the precise condition needed to use it [10]. In part, this is because some papers emphasize different aspects, such as the asymptotic expansion, the replacement of the requirement of nondegenerate ground state by a spectral projection separated from the rest of the spectrum, dependence of first order estimates on the spectral gap, and even extensions to systems without a gap. AT without gap conditions is known to be true [7]; however, in general, no estimates on the error terms are available. J. E. Avron and A. Elgart have shown in Ref.[7] that the AT holds provided the spectral projection is of finite rank independently of any spectral considerations, and that it is much more appropriate for the systems without a gap condition and which have a discrete origin. A similar result was proven in [11] for discrete Hamiltonian when the set of eigenvalues crossings is of measure zero in time. The limitation of these approaches is that, in general, no estimate can be made on the rate at which the adiabatic regime is attained [7].

In this Letter, (i) we present a straightforward, yet rigorous, proof of the AT and AA for systems whose Hamiltonian has a completely continuous spectrum (CS) supposed nondegenerated for reasons of simplicity and which checks a certain number of conditions which will be given later on, (ii) we give a generalization of the GP, (iii) we apply this theory to two physical examples.

In the case of CS we cannot numerate eigenvalues and eigenfunctions, they are characterized by the value of the physical quantity in the corresponding state. Although the eigenfunctions $\varphi(k;t)$ of the operators with CS cannot be normalized in the usual manner as is done for the functions of discrete spectra, one can construct with the $\varphi(k;t)$ new quantities—theWeyl's *eigendifferentials (wave packets)*—[12] which possess the properties of the eigenfunction of discrete spectrum. The eigendifferentials are defined as

$$|\delta\varphi(k;t)\rangle = \int_k^{k+\delta k}|\varphi(k';t)\rangle dk'. \tag{2}$$

They divide up the CS of the eigenvalues into finite but sufficiently small discrete regions of size δk. The eigendifferential (2) is a special wave packet which has only a finite extension in space; hence, it vanishes at infinity and therefore can be seen in analogy to bound states. Furthermore, because the $\delta\varphi$ have finite spatial extension,

they can be normalized. Then in the limit $\delta k \to 0$, a meaningful normalization of the function φ themselves follows: the normalization on δ functions.

For δk, a small connected range of values of the parameter k (this corresponds to a group of "neighboring" states), the operator

$$\delta P(k;t) = \int_k^{k+\delta k} |\varphi(k';t)\rangle\langle\varphi(k';t)| dk' \tag{3}$$

represents the projector (the differential projection operator) onto those states contained in the interval and characterized by the values of the parameter k within the range of values δk. The action of $\delta P(k;t)$ on a wave function $|\psi(t)\rangle$ causes thus the projection of the wave function onto the domain of states $\varphi(k;t)$ which is characterized by k values within the δk interval. Before proceeding further, we give the statement of the AT.

Let us call $U_T(s)$ the evolution operator where s is the fictitious time and T is the time interval during which the evolution of the system takes place and where the slowly time-dependent Hamiltonian $H(s) = \int E(k,s)|\varphi(k,s)\rangle \times \langle\varphi(k,s)| dk$, $0 \le s \le 1$, has a purely CS $E(k,s)$.

If the following conditions are fulfilled (i) As mentioned earlier, the CS is divided into discrete regions of size δk, we must define a gap of energy for the CS; in other words, the size δk is chosen so that $|E(k;s) - E(k';s)| \gg \frac{1}{T}$, $\forall\ k' \notin [k, k+\delta k]$. (ii) We assume that the eigenvalues are piecewise differentiable in the parameter s, and there is no level crossing throughout the transition, i.e., $E(k';s) \neq E(k'';s)/s \in [0,1]$, $k' \in [k, k+\delta k]$, $k'' \notin [k, k+\delta k]$. (iii) The derivatives $\frac{\partial}{\partial s}\delta P(k;s)$ and $\frac{\partial^2}{\partial s^2}\delta P(k;s)$ are well defined and continuous in the interval $0 \le s \le 1$.

Under these conditions, it is possible to prove the AT:

Theorem.—If the quantum system with time-dependent Hamiltonian having a nondegenerate CS is initially in an eigenstate $|\varphi(k,0)\rangle$ of $H(0)$ and if $H(s)$ evolves slowly enough, then the state of the system at any time s will remain in the interval $[k, k+\delta k]$.

The AT can be formally written, at the first order, in terms of the evolution operator as

$$\forall\ k: \lim_{T\to\infty} U(s)\delta P(k;0) = \delta P(k;s) \lim_{T\to\infty} U(s) + O\left(\frac{1}{T}\right). \tag{4}$$

Notice that if, initially, the system is in the state $|\varphi(k,0)\rangle$ so that $H(0)|\varphi(k,0)\rangle = E(k,0)|\varphi(k,0)\rangle$ and expanding an arbitrary state vector on the basis of the instantaneous quasi-eigenfunction, then in the limit $T \to \infty$ (4) implies that the state

$$|\psi(s)\rangle = U(s)|\varphi(k;0)\rangle = \int_k^{k+\delta k} C_{k'}(s)|\varphi(k';s)\rangle dk', \tag{5}$$

belongs to the subspace generated by the states $|\varphi(k;s)\rangle$ pertaining to the interval $[k, k+\delta k]$.

Proof.—The demonstration that we present follows the same approach developed in Ref. [12] for the discrete case, and it consists of three steps: first, we change to the evolution picture where the Hamiltonian has time-dependent spectral projections; i.e., we go over to a time-dependent reference frame following the axes which diagonalize $H(s)$. In this picture, the time evolution generator contains an immediately integrable contribution, which we eliminate by going over to a second picture, and finally, one shows that the remaining evolution operator differs from identity by terms $O(1/T)$. We introduce a unitary transformation $U_T(s) = A(s)\Phi_T(s)W(s)$ where the unitary operator $A(s)$ has the property $\delta P(k,s) = A(s)\delta P(k,0)A^+(s)(\forall\ k \in \mathbb{R})$ and is completely defined by the initial condition $A(0) = I$ and the differential equation $i\hbar\partial A(s)/\partial s = K(s)A(s)$. The appropriate Hermitian operator $K(s)$ obeys the following commutation relation,

$$i\hbar\frac{\partial}{\partial s}\delta P(k,s) = [K(s), \delta P(k,s)], \tag{6}$$

and is determined without ambiguity if we add the additional condition $\langle\varphi(k;t)|K(t)|\varphi(k';t)\rangle = 0$, $(\forall\ k' \in [k, k+\delta k])$. This gives

$$K(t) = i\hbar\int[1 - \delta P(k;t)]|\dot\varphi(k;t)\rangle\langle\varphi(k;t)| dk. \tag{7}$$

The unitary transformation $A^+(s)$ carries the vectors and operators of the Schrödinger "representation" over the vectors and operators of a new "representation," the "rotating axis representation." The observable $H(s)$ is transformed into $H^{(A)}(s) = A^+(s)H(s)A(s)$ giving $H^{(A)}(s) = \int E(k,s)|\varphi(k,0)\rangle\langle\varphi(k,0)| dk$. Similarly, $K(s)$ becomes $K^{(A)}(s) = A^+(s)K(s)A(s)$. The operator $\Phi_T(s)$ may be written, with the initial condition $\Phi_T(0) = I$, as

$$\Phi_T(s) = \int e^{-(i/\hbar)T\alpha(k,s)}|\varphi(k,0)\rangle\langle\varphi(k,0)| dk, \tag{8}$$

where $\alpha(k,s) = \int_0^s E(k,s')ds'$. The demonstration of (4) is equivalent to showing that $[W(s), \delta P(k,0)] = 0$. To prove this result, we insert $U_T(s)$ in the evolution equation $i\hbar\partial U_T(s)/\partial s = TH(s)U_T(s)$. This gives the equation satisfied by the unitary operator W in its integral form

$$W(s) = I + \frac{i}{\hbar}F(s)W(s) + \frac{1}{\hbar^2}\int_0^s F(s')\bar K(s)W(s')ds', \tag{9}$$

taking into account the equation $i\hbar\partial W(s)/\partial s = \bar K(s)W(s)$ and $F(s) = \int_0^s \bar K(s')ds'$ where $\bar K(s) = \Phi_T^+(s)K^{(A)}(s)\Phi_T(s)$. We are going to show that $F(s)$ is a sum of oscillating functions whose frequencies increase indefinitely with T, and consequently, the two last terms on the right-hand side of the equation (9) tend to zero when $T \to \infty$. Any operator [and in particular $F(s)$] admits the following decomposition $F(s) = \iint F(k,k',s)dkdk' = \int_0^s P(k,0)\bar K(s')P(k',0)ds'$, where $P(k,0) = I$ is the projector. Using (8), we obtain

$$F(k,k',s) = \int_0^s \exp\left[\frac{i}{\hbar}T[\alpha(k,s') - \alpha(k',s')]\right] \times K^{(A)}(k,k',s')ds' \tag{10}$$

where $k' \notin [k, k+\delta k]$, because for $k' \in [k, k+\delta k]$, the $F(k,k',s)$ vanish (see the condition stated above). $K^{(A)}(k,k',s')$ is a continuous function of s independent of T. The phase of the exponential, however, does depend on

T, and $F(k, k', s)$ is therefore of the form $\int_0^s e^{iT\alpha(s')/\hbar} f(s')ds'$, where f is a continuous function and α is a continuous monotonic function. Such an integral is known to go to zero when $T \to \infty$. In conclusion, when $T \to \infty$ we have $F(s) = O(1/T)$. Since the two last terms in Eq. (9) contain the factor $F(s)$, then for $T \to \infty$ and from $U_T(s) = A(s)\Phi_T(s)W(s)$, we obtain

$$U_T(s) \simeq A(s)\Phi_T(s)\left[I + O\left(\frac{1}{T}\right)\right]. \quad (11)$$

Finally, (8) implies $\Phi_T(s)\delta P(k, 0) = \delta P(k, 0)\Phi_T(s)$ and hence $A(s)\Phi_T(s)\delta P(k,0) = A(s)\delta P(k,0)\Phi_T(s) = \delta P(k,s) \times A(s)\Phi_T(s)$. This concludes the proof of the AT (4). ■

If T is sufficiently large, we can, in first approximation, replace $U(t_1, t_0)$ by its asymptotic form:

$$U(t_1, t_0) = U_T(1) \simeq A(1)\Phi_T(1). \quad (12)$$

This is called the AA. If the initial normalized state is $|\varphi(k_0, 0)\rangle$, then under this approximation, $U(t_1, t_0)|\varphi(k_0, 0)\rangle \approx A(1)\Phi_T(1)|\varphi(k_0, 0)\rangle$. To determine the validity of the AA for a given process, we can estimate the error by computing the probability $\eta = \langle\varphi(k_0, 0)|W^+(1)Q_0W(1)|\varphi(k_0, 0)\rangle$ of finding the system at time t_1 in a state different from $A(1)\Phi_T(1)|\varphi(k_0, 0)\rangle$, where $Q_0 = I - \delta P(k_0, 0)$. Solving (9) iteratively and keeping only the first order term, we find

$$\eta \approx \frac{1}{\hbar^2}\int_{k\notin[k_0,k_0+\delta k_0]} |\langle\varphi(k_0, 0)|F(1)|\varphi(k, 0)\rangle|^2 dk. \quad (13)$$

Hence, the AA is applicable when $\eta \ll 1$. This condition is not easy to verify in practice because in general we do not have enough explicit information about the operator $F(1)$. A different way of writing $\eta \ll 1$, more amenable to interpretation, is to define a normalized time through the variable transformation $t = t_0 + sT$ $(0 \le s \le 1)$, and the initial normalized state $|\varphi(k_0, t_0)\rangle$ of $H(t_0)$ with the eigenvalue $E(k_0, t_0)$. Then, using (7) and (10) and performing the change $s \to t$ in (13) yields

$$\eta \approx \frac{1}{\hbar^2}\int_{k\notin[k_0,k_0+\delta k_0]} \left| i\hbar \int_{t_0}^{t_1} e^{(i/\hbar)\int_{t_0}^{t}[E(k_0,t')-E(k,t')]dt'} \langle\varphi(k_0, t)|\dot{\varphi}(k, t)\rangle dt \right|^2 dk. \quad (14)$$

The condition $\eta \ll 1$ is, therefore, in most cases, certainly satisfied if

$$\max_{k\notin[k_0,k_0+\delta k_0]} |\langle\varphi(k_0, t)|\dot{\varphi}(k, t)\rangle| \ll \min_{k\notin[k_0,k_0+\delta k_0]} |E(k_0, t') - E(k, t')|, \quad \forall\, t \in [t_0, t_1], \quad (15)$$

with max and min taken over all $k \notin [k_0, k_0 + \delta k_0]$. Condition (15) may be taken as a criterion for the validity of the AA in the case of a CS. This estimate of the AA could not be derived if using the Avron-Elgart's approach [7] as mentioned earlier.

The question arises: is there a GP for a CS? This case was raised for the first time by R. G. Newton [13] who looks at the S matrix as a GP factor. Newton introduced what may be called the noninteraction picture to get the GP factor in the CS. G. Ghosh [13] extends the AA to the continuous spectra like an ansatz.

In order to derive the GP for the nondegenerate CS, we insert (5) in the Schrödinger equation (1) and we multiply the resulting equation by $\int_{-\infty}^{+\infty}\langle\varphi(k''; t)|dk''$, since k can sweep all the possible values and the intervals δk should be small $(\delta k \to 0)$ the equality between integrals implies the equality between integrands, this yields

$$C_k(t) = \delta(k' - k) \times e^{-\int_{t_0}^{t}[(i/\hbar)E(k';t')+\int_{-\infty}^{+\infty} dk''\langle\varphi(k'';t')|(\partial/\partial t')|\varphi(k';t')\rangle]dt'}; \quad (16)$$

hence, the adiabatic solution of the time-dependent Schrödinger equation (1) is

$$|\psi(k, t)\rangle = e^{(i/\hbar)[-\gamma^D(k;t)+\gamma^G(k;t)]}|\varphi(k; t)\rangle, \quad (17)$$

where $\gamma^D(k; t)$ is the familiar dynamical phase factor, and

$$\gamma^G(k; t) = \int_{t_0}^{t}\int_{-\infty}^{+\infty}\langle\varphi(k'; t')|i\hbar\frac{\partial}{\partial t'}|\varphi(k; t')\rangle dt'dk', \quad (18)$$

is the generalized GP which embodies another central result of this Letter. Note that all properties of the GP in discrete case are fulfilled by the generalized GP $\gamma^G(k; t)$ (18) for the continuous case.

We now want to analyze the nature of the phase (18) through examples. Our first case is the Dirac equation in a time-dependent electromagnetic field where the Hermitian time-dependent Dirac Hamiltonian defined in a 4-dimensional Hilbert space spanned by the two-dimensional basis state $|1\rangle$ and $|2\rangle$ can be written

$$H_D(t) = m(t)c^2[|1\rangle\langle 1| - |2\rangle\langle 2|] + c\sigma^3[p - f(t)]|1\rangle\langle 2| + c\sigma^3[p - f^*(t)]|2\rangle\langle 1| \quad (19)$$

p is the momentum operator, the mass $m(t)$ and $f(t)$ are periodic slow functions of time, σ^3 is the 2×2 standard Pauli matrix. At any time t, the instantaneous eigenstates (normalized to δ function) of the Hamiltonian (19) are

$$|\varphi^{\pm}(z, k; t)\rangle = \left\{\frac{c\sigma^3 g(k;t)}{\sqrt{[m(t)c^2 \mp \hbar\omega(k;t)]^2 + |g(k;t)|^2c^2}}|1\rangle + \frac{m(t)c^2 \mp \hbar\omega(k;t)}{\sqrt{[m(t)c^2 \mp \hbar\omega(k;t)]^2 + |g(k;t)|^2c^2}}|2\rangle\right\} \times \frac{e^{(i/\hbar)kz}}{\sqrt{2\pi\hbar}} \quad (20)$$

and correspond to the eigenvalues $\pm\hbar\omega(k, t)$ where $\hbar\omega(k; t) = c\sqrt{m^2(t)c^2 + |g(k; t)|^2}$ and $g(k; t) = f(t) - k$. Substituting (20) in Eq. (18) and using of the following

representation of the adiabatic parameters $[\mathrm{Re}f(t) - k]c = \hbar\omega\sin\theta\cos\varphi$, $\mathrm{Im}f(t)c = \hbar\omega\sin\theta\sin\varphi$ and $m(t)c^2 = \hbar\omega\cos\theta$; ω, θ, and φ are now chosen as time-dependent adiabatic quantities, we find that the generalized GP is nothing but the solid angle $\gamma^G(k; C) = -\frac{\hbar}{2}\Omega$ subtended by the circuit C when seen from $(k, 0, 0)$ in $[\mathrm{Re}f(t), \mathrm{Im}f(t), m(t)c]$ space.

Our next example is the geometrical aspect of the S matrix: A very general way of looking at the S matrix as a GP factor has been implicitly provided by Newton [13], where the expression for GP looks strikingly similar to the equation of the wave operator in the interaction picture. This leads Newton to conclude that the S matrix appears in geometric phase as an expression of the adiabatic switching on and off of the interaction. Here, we show explicitly that, in the case of an elastic scattering, the generalized GP (18) is nothing but the diagonal element of the S matrix.

The state vector $|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$ of the given physical system is assumed to satisfy the Schrödinger equation (1), $U(t, t_0)$ being the unitary evolution operator associated to the Hamiltonian operator $H(t)$. In order to solve Eq. (1) under the adiabatic assumption, we assume that the Hamiltonian can be split into two parts $H(t) = H_0 + V(t)$ so that H_0 represents the noninteracting particles Hamiltonian . In other words, H_0 represents the free Hamiltonian operator whose eigenstates in the CS are defined as $H_0|\varphi^F(k)\rangle = E(k)|\varphi^F(k)\rangle$. For the present, we have primarily elastic scattering in mind, and we may think of $V(t)$ as the time-dependent potential of interaction. We assume that $V(t)$ varies slowly in time with $V(t) \neq 0$ for $t_0 < t < t_1$.

In scattering problems, we are interested in calculating transition amplitudes between states $|\varphi^F(k)\rangle$ (F stands for free evolution). The system initially in the state $|\psi(-\infty)\rangle = |\varphi^F(k_0)\rangle$ evolves freely towards the interaction region under the action of the free Hamiltonian H_0. Expansion of the adiabatic evolved state $|\psi(t)\rangle$ (17) on the basis of the instantaneous eigenstates $|\varphi^F(k)\rangle$ of H_0 leads to the matrix elements of the evolution operator $U(t, t_0)$ in the basis $\{|\varphi^F(k)\rangle\}$

$$\langle\varphi^F(k)|U(t, t_0)|\varphi^F(k_0)\rangle = e^{(i/\hbar)[-\gamma^D(k_0;t)+\gamma^G(k_0;t)]}\langle\varphi^F(k)|\varphi(k_0; t)\rangle. \quad (21)$$

In the interaction picture $\tilde{U}(t, t_0) = e^{\frac{i}{\hbar}(t-t_0)H_0}U(t, t_0)$, the corresponding matrix elements of $\tilde{U}$ between the eigenstates of the unperturbed Hamiltonian H_0 satisfy

$$\langle\varphi^F(k)|\tilde{U}(t, t_0)|\varphi^F(k_0)\rangle = e^{(i/\hbar)[-\gamma^D(k_0;t)+\int_{t_0}^{t}E(k)dt'+\gamma^G(k_0;t)]}\langle\varphi^F(k)|\varphi(k_0; t)\rangle. \quad (22)$$

As expected, the initial ($t \leq t_0$) and final ($t \geq t_1$) eigenstates of the free Hamiltonian H_0 are identical, i.e., $|\varphi^F(k_0, t \geq t_1)\rangle = |\varphi^F(k)\rangle$. By pushing the initial time into the distant past, i.e., $t_0 \to -\infty$, similarly $t \to \infty$ signals that the scattering process is complete, we obtain the scattering matrix or S matrix

$$\langle\varphi^F(k)|S|\varphi^F(k_0)\rangle = \delta(k - k_0)\exp\left[\frac{i}{\hbar}\gamma^G(k_0; +\infty)\right]. \quad (23)$$

On the basis of this comparison, we may conclude that after the Hamiltonian completes an adiabatic circuit from H_0 via $H(t)$ back to H_0, the state which initially was given by $|\varphi^F(k)\rangle$ has gone over into a new state that differs from it by a multiplicative factor S_k which is the eigenvalue of the unitary S matrix; it is related to the generalized GP (18) by $S_k = \exp[\frac{i}{\hbar}\gamma^G(k; +\infty)]$.

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