Adiabatic Theorem in the Case of Continuous Spectra

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Abstract

In this paper, we present a rigorous demonstration and discussion of the quantum adiabatic theorem for systems having a non-degenerate continuous spectrum. A new strategy is initiated by defining a kind of gap, "a virtual gap", for the continuous spectrum through the notion of eigendifferential (Weyl’s packet) and using the differential projector operator. Finally, we obtain the validity condition of the adiabatic approximation.

PACS: 03.65.Ca, 03.65.Ta

The adiabatic theorem is one of the basic results in quantum theory [1, 2]. It is concerned with quantum systems described by an explicitly, but slowly, time-dependent Hamiltonian. There has been a sudden regain of interest in the adiabatic theorem for itself among physicists when in 1984 M. V. Berry [3] pointed out that if it was applied to Hamiltonians satisfying \( H(t_1) = H(t_2) \), it could generate a phase factor having non-trivial geometrical meaning. And more recently, the adiabatic theorem has renewed its importance in the context of quantum control [4], for example, concerning adiabatic passage between atomic energy levels, as well as for adiabatic quantum computation [5].

There are several points of view for a discussion of the quantum adiabatic theorem; each one offers interesting insight. As T. Kato [2] has pointed out, the contents of the adiabatic theorem embody two parts: first, the existence of a virtual change of the system which may be called an adiabatic transformation, and, second, the dynamical transformation of the system goes over to an adiabatic transformation in the limit when the change of the Hamiltonian is infinitely slow. The adiabatic theorem proof given by M. Born and V. Fock [1], although very general, is still restricted by the assumption of considering the purely discrete and non-degenerate Hamiltonian’s spectrum, except for accidental degeneracy caused by crossing. These limitations are rather artificial from the physical point of view and should be removed from Kato’s derivation of the adiabatic theorem. Several authors [6] had formally extended the Kato’s results on the approximate validity of the adiabatic theorem when the time \( T \), during which the approximation takes place, is large but finite. G. Nenciu [7] demonstrated the adiabatic theorem for bounded Hamiltonians. Later, J. E. Avron and A. Elgart [8] showed that the adiabatic theorem holds for unbounded Hamiltonians as well and applied it to deal with the quantum Hall effect.

Let us simply recall here that the works following that of Born and Fock [1] by Kato [2], Garrido [6], Nenciu [7] and J. E. Avron et al. [7] have led to a formulation of the adiabatic theorem 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 \( \min_{0 \leq t \leq T} g_{nm}(t) \) the smaller will be the transition probability.

Despite the existence of extensive literature on rigorous proofs of estimates needed to justify the adiabatic approximation [2,7,8,9], doubts have been raised about its validity [10] leading to confusion about the precise condition needed to use it [11]. In part, this is because some papers emphasize different aspects, such as the asymptotic expansion, the replacement of the requirement of non-degenerate 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. Adiabatic theorem without gap conditions is know to be true [5], however, in general, no estimates on the error terms are available. J. E. Avron and A. Elgart have shown in ref. [8] that the adiabatic theorem holds provided the spectral projection is of finite rank independently of any spectral considerations. A similar result was proven by F. Bornemann [12] 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 [8]. The gap condition is generally
associated to spectral stabilities. Consequently, the situation where the gap does not exist will led to spectral instabilities. Thus it is difficult to establish smooth spectral projections which is a necessary condition for the validity of the adiabatic theorem in the practical applications. In fact, the generalized adiabatic theorem, according to J. E. Avron and A. Elgart’s approach [8], is much more appropriate for the systems without a gap condition and which have a discrete origin.

In this letter, we present a straightforward, yet rigorous, proof of the adiabatic theorem and adiabatic approximation for systems whose Hamiltonian has a completely continuous spectrum supposed non-degenerated for reasons of simplicity and which checks a certain number of conditions which will be given later on.

In the case of continuous spectrum we cannot numerate eigenvalues and eigenfunctions, they are characterised by the value of the physical quantity in the corresponding state. Although the eigenfunctions \( \varphi (k; t) \) of the operators with continuous spectra cannot be normalised in the usual manner as is done for the functions of discrete spectra, one can construct with the \( \varphi (k; t) \) new quantities - the Weyl’s eigendifferentials (wave packets) [13] which possess the properties of the eigenfunction of discrete spectrum. The eigendifferentials are defined by the equation

\[
| \delta \varphi (k; t) \rangle = \int \frac{k + \delta k}{k} | \varphi (k'; t) \rangle \, dk'.
\] (1)

They divide up the continuous spectrum of the eigenvalues into finite but sufficiently small discrete regions of size \( \delta k \) (see Fig. 1).

Figure 1: Decomposition of the continuous spectrum.

The eigendifferential [13] 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 \( \varphi \) themselves follows: the normalization on \( \delta \) functions.

For \( \delta k \), a small connected range of value of the parameter \( k \) (this corresponds to a group of “neighboring” states, see Fig 1), the operator

\[
\delta P (k; t) = \int \frac{k + \delta k}{k} | \varphi (k'; t) \rangle \langle \varphi (k'; t) | \, dk'.
\] (2)

represents the projector (the differential projection operator [14]) onto those states contained in the interval and characterized by the values of the parameter \( k \) within the range of values \( \delta k \). The action of \( \delta P (k; t) \) on a wavefunction \( | \psi (t) \rangle \) is defined by

\[
\delta P (k; t) | \psi (t) \rangle = \int \frac{k + \delta k}{k} | \varphi (k'; t) \rangle \langle \varphi (k'; t) | \, dk'.
\] (3)

The application of the differential projection operator \( \delta P (k; t) \) causes thus the projection of the wavefunction onto the domain of states \( \varphi (k; t) \) which is characterized by \( k \) values within the \( \delta k \) interval. Before proceeding further, we give the statement of the adiabatic theorem.
Figure 2: Evolution of a range of energy of width \( \delta k \) as a function of time.

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

\[
i\hbar \frac{\partial}{\partial s} U_T(s) = TH(s)U_T(s),
\]

and the slowly time-dependent Hamiltonian \( H(s) = \int E(k,s)|\varphi(k,s)\rangle\langle\varphi(k,s)| dk \), \( 0 \leq s \leq 1 \), has a purely continuous spectrum \( E(k,s) \).

If the following conditions are fulfilled

(i) As it is mentioned earlier (see Fig.1) the continuous spectrum is divided into discrete regions of size \( \delta k \), we must define or create a gap of energy for the continuous spectrum, in other words, the size \( \delta k \) is chosen so that

\[
E(k;s) - E(k';s) \gg \frac{1}{T}, \quad \forall k' \notin [k, k + \delta k].
\]

(ii) We assume that the eigenvalues are piecewise differentiable in the parameter \( s \), and there is no level crossing throughout the transition (see Fig.2), in other words:

\[
E(k';s) \neq E(k'';s) \quad / s \in [0, 1], k' \in [k, k + \delta k], \quad k'' \notin [k, k + \delta k].
\]

(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 \( 0 \leq s \leq 1 \).

Under these conditions it is possible to prove the adiabatic theorem:

**Theorem 1** If the quantum system with time-dependent Hamiltonian having a non degenerate continuous spectrum 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 adiabatic theorem can be formally written, at the first order, in terms of the evolution operator as

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

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 (7) implies

\[
\lim_{T \to \infty} U(s) |\varphi(k,0)\rangle = \delta P(k;s) \lim_{T \to \infty} U(s) |\varphi(k,0)\rangle
\]

and in the limit \( T \to \infty \) the state \( U(s)|\varphi(k,0)\rangle = \int_{k}^{k+\delta k} C(k';s)|\varphi(k';s)\rangle dk' \), belongs to the subspace generated by the states \( |\varphi(k;s)\rangle \) pertaining to the interval \([k, k + \delta k]\).
We go over to a second picture and we show that the remaining evolution operator differs from the identity by

$$\delta P (k, s) = A (s) \delta P (k, 0) A^+ (s) \quad \forall k \in \mathbb{R}. \tag{9}$$

It is completely defined by the initial condition $A (0) = I$ and the differential equation

$$i\hbar \frac{\partial}{\partial s} A (s) = K (s) A (s). \tag{10}$$

The operator $K (s)$ obeys the following commutation relation:

$$i\hbar \frac{\partial}{\partial s} \delta P (k, s) = [K (s), \delta P (k, s)], \tag{11}$$

and is determined without ambiguity if we add the following supplementary condition:

$$\langle \varphi (k; t) | K (t) | \varphi (k'; t) \rangle = 0, \quad \forall k' \in [k, k + \delta k], \tag{12}$$

equation that yields the following expression

$$K (t) = i\hbar \int [1 - \delta P (k; t)] | \dot{\varphi} (k; t) \rangle \langle \varphi (k; t) | dk. \tag{13}$$

The unitary transformation $A^+ (s)$, applied to the operators and the vectors of the Schrödinger’s picture, produces a new picture: the rotating axis picture:

$$H^{(A)} (s) = A^+ (s) H (s) A (s) = \int E (k, s) | \varphi (k, 0) \rangle \langle \varphi (k, 0) | dk, \tag{14}$$
similarly $K^{(A)} (s)$ becomes

$$K^{(A)} (s) = A^+ (s) K (s) A (s). \tag{15}$$

The evolution operator in this new "representation" is $U^{(A)} (s) = A (s) U_T (s)$. It is defined by

$$i\hbar \frac{\partial}{\partial s} U^{(A)} (s) = \left[ TH^{(A)} (s) - K^{(A)} (s) \right] U^{(A)} (s), \quad U^{(A)} (0) = I. \tag{16}$$

Since $H^{(A)} (s)$ and $K^{(A)} (s)$ are $T$-independent, it is to be expected that in the $T \to \infty$ limit the first term of the right hand side in (15) dominates. We can approximately solve such an equation in which we go over to a time-dependent reference frame following the axis which diagonalize $H^{(A)} (s)$. We define $\Phi_T (s)$ via

$$i\hbar \frac{\partial}{\partial s} \Phi_T (s) = TH^{(A)} (s) \Phi_T (s), \tag{17}$$
in which the solution may be written, with the initial condition $\Phi_T (0) = I$, as

$$\Phi_T (s) = \exp \left[ \int_0^s \frac{i T \alpha (k, s')}{\hbar} \right] | \varphi (k, 0) \rangle \langle \varphi (k, 0) | dk, \tag{18}$$

where $\alpha (k, s) = \int_0^s E (k, s') ds'$. If, as we will see immediately, $U^{(A)} (s)$ tends toward $\Phi_T (s)$ for large $T$, we will have approximately

$$U_T (s) \approx \Phi_T (s). \tag{19}$$

We go over to a second picture and we show that the remaining evolution operator differs from the identity by terms $O (\frac{1}{T})$. Thus, we change to a last picture with operator $W (s) \equiv \Phi_T^+ (s) A^+ (s) U_T (s)$, and $(-)$ generator $K (s) = \Phi_T^+ (s) A^+ (s) K (s) A (s) \Phi_T (s):

$$i\hbar \frac{\partial}{\partial s} W (s) = K (s) W (s), \quad W (0) = I, \tag{20}$$
equivalent to the integral equation

$$W (s) = I + \frac{i}{\hbar} \int_0^s K (s') W (s') ds'. \tag{21}$$
Now, we prove that in the limit $T \to \infty$, $W(s) = I + O\left(\frac{1}{T}\right)$. We begin by considering the operator $F(s) = \int_0^s \bar{K}(s') \, ds'$. Any operator (and in particular $F(s)$) admits the following decomposition

$$F(s) = \int \int F(k, k', s) \, dk \, dk'$$

$$= \int_0^s \int \langle \varphi(k,0) | \bar{K}(s') | \varphi(k',0) \rangle \langle \varphi(k,0) | \varphi(k',0) \rangle \, dk \, dk' \, ds'.$$

Using (18) we obtain:

$$F(k, k', s) = \int_0^s \exp \left[ \frac{iT}{\hbar} \left( \alpha(k, s') - \alpha(k', s') \right) \right] \frac{K^{(A)}(k, k', s')}{E(k, s') - E(k', s')} \, ds', \quad k' \notin [k, k + \delta k], \tag{22}$$

an expression in which we have introduced the condition $k' \notin [k, k + \delta k]$ because, from (12), we deduce $F(k, k', s) = 0$ for $k' \in [k, k + \delta k]$.

Let $k' \notin [k, k + \delta k]$, since $K^{(A)}(k, k', s')$ is a continuous function of $s$, our assumption implies that $\alpha(k, s') - \alpha(k', s')$ is a continuous nonvanishing monotonic function of $s$; after integrating (23) by parts we obtain

$$F(k, k', s) = \frac{\hbar}{iT} \left[ \exp \left[ \frac{iT}{\hbar} \left( \alpha(k, s') - \alpha(k', s') \right) \right] \frac{K^{(A)}(k, k', s')}{E(k, s') - E(k', s')} \right]_{0}^{s} -$$

$$- \int_0^s \exp \left[ \frac{iT}{\hbar} \left( \alpha(k, s') - \alpha(k', s') \right) \right] \frac{\partial}{\partial s} \left[ \frac{K^{(A)}(k, k', s')}{E(k, s') - E(k', s')} \right] \, ds', \tag{24}$$

hence, according to the condition (15), $F(k, k', s), k' \notin [k, k + \delta k]$, asymptotically converges toward 0 as $\frac{1}{T}$.

Summarizing, as $T \to \infty$ we have:

$$F(s) = O\left(\frac{1}{T}\right). \tag{25}$$

Using (20), integration by parts turns (21) into:

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

since the last two terms in this equation contain the factor $F(s)$, then for $T \to \infty$ and from $U_T(s) = A(s) \Phi_T(s) W(s)$ we obtain

$$U_T(s) \simeq A(s) \Phi_T(s) \left[ I + O\left(\frac{1}{T}\right) \right], \tag{27}$$

Finally (18) implies $\Phi_T(s) \delta P(k, 0) = \delta P(k, 0) \Phi_T(s)$ and hence $A(s) \Phi_T(s) \delta P(k, 0) = A(s) \delta P(k, 0) \Phi_T(s) = \delta P(k, s) A(s) \Phi_T(s)$. This concludes the proof of the adiabatic theorem (17).

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

$$U(t_1, t_0) = U_T(1) \simeq A(1) \Phi_T(1). \tag{28}$$

This is called the adiabatic approximation. If the initial normalized state is $|\varphi(k_0, 0)\rangle$, 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 adiabatic approximation for a given process, we can estimate the error by computing the probability $\eta$ of finding the system at time $t_1$ in a state different from $A(1) \Phi_T(1) |\varphi(k_0, 0)\rangle$:

$$\eta = \langle \varphi(k_0, 0) | U^+(t_1, t_0) A(1) \Phi_T(1) Q_0 A^+(1) \Phi_T^+(1) U(t_1, t_0) | \varphi(k_0, 0) \rangle,$$

where $Q_0 = I - \delta P(k_0, 0)$. This quantity may be rewritten as

$$\eta = \langle \varphi(k_0, 0) | W^+(1) Q_0 W(1) | \varphi(k_0, 0) \rangle.$$

Solving (24) iteratively and keeping only the first order term, we find

$$\eta \approx \frac{1}{\hbar^2} \langle \varphi(k_0, 0) | F^+(1) Q_0 F(1) | \varphi(k_0, 0) \rangle$$

$$= \frac{1}{\hbar^2} \int_{k \notin [k_0, k_0 + \delta k]} |\langle \varphi(k_0, 0) | F(1) | \varphi(k_0, 0) \rangle|^2 \, dk. \tag{31}$$
Now, let us define a normalized time through the variable transformation $t = t_0 + sT$ ($0 \leq s \leq 1$), 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 (33), (29) and performing the change $s \to t$ in eq. (31) yields

$$\langle \varphi(k_0, t_0) | F(t_1) | \varphi(k, t_0) \rangle = i\hbar \int_{t_0}^{t_1} \exp \left\{ \frac{i}{\hbar} \int_{t_0}^{t} [E(k_0, t') - E(k, t')] dt' \right\} \langle \varphi(k_0, t) | \varphi(k, t) \rangle dt.$$  

(32)

Since $\langle \varphi(k_0, t) | \delta P(k_0, t) | \varphi(k, t) \rangle = 0$ for $k \notin [k_0, k_0 + \delta k_0]$ equation (31) may be recast as

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

(33)

and the adiabatic approximation for $|\varphi(k_0, t_0)\rangle$ holds only if $\eta \ll 1$ which requires

$$\delta \psi(k_0 \to k, t) = \left| i\hbar \int_{t_0}^{t_1} \exp \left\{ \frac{i}{\hbar} \int_{t_0}^{t} [E(k_0, t') - E(k, t')] dt' \right\} \langle \varphi(k_0, t) | \varphi(k, t) \rangle dt \right|^2 \ll 1, \quad \forall k \notin [k_0, k_0 + \delta k_0],$$  

(34)

the integral of eq. (33) will be sufficiently small, if the phase of the integrated function vibrates fast enough and the amplitude of the integrated function is small enough, thus $\delta \psi(k_0 \to k, t)$ is at the maximum

$$\delta \psi(k_0 \to k, t) \approx \max_{t \in [t_0, t_1]} \left| \frac{\hbar}{E(k_0, t') - E(k, t')} \frac{\langle \varphi(k_0, t) | \varphi(k, t) \rangle}{\langle \varphi(k_0, t) | \varphi(k, t) \rangle} \right|^2, \quad \forall k \notin [k_0, k_0 + \delta k_0].$$  

(35)

The condition $\eta \ll 1$ is therefore, in most cases, certainly satisfied if $\max_{k \notin [k_0, k_0 + \delta k_0]} \delta \psi(k_0 \to k, t) \ll 1$ or equivalently,

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

(36)

with max and min taken over all $k \notin [k_0, k_0 + \delta k_0]$. Condition (36) may be taken as a criterion for the validity of the adiabatic approximation in the case of a continuous spectrum. This estimate of the adiabatic approximation could not be made in the Avron-Elgart’s approach [5] as mentioned earlier.

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