The Adiabatic Theorem for Quantum Systems with Spectral Degeneracy

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By stating the adiabatic theorem of quantum mechanics in a clear and rigorous way, we establish a necessary condition and a sufficient condition for its validity, where the latter is obtained employing our recently developed adiabatic perturbation theory. Also, we simplify further the sufficient condition into a useful and simple practical test at the expenses of its mathematical rigor. We present results for the most general case of quantum systems, i.e., those with degenerate energy spectra. These conditions are of upmost importance to assess the validity of practical implementations of non-Abelian braiding and adiabatic quantum computation. To illustrate the degenerate adiabatic approximation, and the necessary and sufficient conditions for its validity, we analyze in depth an exactly solvable time-dependent degenerate problem.

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The adiabatic theorem \cite{nota1} has played, and still plays, a fundamental role in practical quantum physics applications. Indeed, the ability to determine how the \textit{slow} dynamics of external probes coupled to a system affect its time evolution has applications ranging from the notion of thermal equilibrium and non-equilibrium phenomena \cite{nota2} to the conditions under which an adiabatic quantum computer can reliably operate \cite{nota2}. Useful and practical quantitative conditions for the validity of the adiabatic theorem are also relevant to the important current problem of assessing the feasibility of any information processing scheme that uses the concept of fractional exchange statistics and non-Abelian braiding \cite{nota3}.

General physical principles dictate that, in three space dimensions, elementary particles can only obey fermionic or bosonic statistics. Kinematic constraints do not allow for fractional exchange statistics: electrons are spin-1/2 fermions and photons are spin-1 bosons. Nonetheless, fractional statistics \textit{particles} or \textit{modes} may emerge from the collective behavior of elementary particles, i.e., collective excitations of a quantum field, as a result of a dynamical process. The latter requires special circumstances and constraints that should be analyzed on a case by case basis. For instance, for two localized degenerate Majorana modes to realize a non-Abelian braiding process we need to design the physical Hamiltonians realizing the braiding that do not lift the degeneracy and can be implemented adiabatically. If those constraints are not met experimentally then the braiding operation is faulty. Physical systems where such fractional statistics emerges have highly degenerate energy spectrum, thus justifying a careful statement of the adiabatic theorem and the precise conditions for its validity.

Despite its practical importance, no consensual and rigorous necessary and sufficient conditions for the validity of the adiabatic theorem have been given. Only recently a proof that the commonly used textbook condition \cite{nota4} is necessary for non-degenerate Hamiltonians \cite{nota6} but not sufficient \cite{nota7} was given. For degenerate systems, even a clear presentation of the theorem is lacking, let alone necessary and sufficient conditions. It is this paper’s intention to fill that gap.

With that in mind, our goal is three fold. First, using techniques developed in \cite{nota8, nota9}, we aim at providing a clear and rigorous version of the adiabatic theorem for Hamiltonians with non-degenerate and degenerate spectra using a single formalism. We want to be as precise as possible in stating the adiabatic theorem to avoid common misunderstandings \cite{nota10}, mainly due to a lack of quantitative rigor in the way the theorem is usually presented. Second, we prove necessary and sufficient conditions for the validity of the rigorous version of the adiabatic theorem here presented. The necessary condition for degenerate spectra reduces to the one in \cite{nota2} when no degeneracy is present. To obtain a sufficient condition, we rely on the adiabatic perturbation theory developed in \cite{nota2, nota3}. Finally, we apply these ideas to an exactly solvable time-dependent degenerate problem \cite{nota6}, where we show that the necessary and sufficient conditions here developed provide the correct conditions under which the adiabatic theorem holds.

To properly formulate the degenerate adiabatic theorem (DAT) we first need to introduce the degenerate adiabatic approximation (DAA). As we will see, DAT is essentially a statement about the mathematical conditions for the validity of DAA. This understanding of the essence of the adiabatic theorem is akin to the ones of Berry \cite{nota11} and Tong \cite{nota12}, for non-degenerate systems, and to the ones of Wilczek and Zee \cite{nota11} and Wilczek \cite{nota12}, for degenerate systems.

\textit{Degenerate Adiabatic Approximation}. Consider an explicitly time-dependent Hamiltonian $H(t)$ with orthonormal eigenvectors $|n^{\beta_n}(t)\rangle$, where $g_n = 0, 1, \ldots, d_n - 1$ labels states of the degenerate eigenspace $\mathcal{H}_n$ of dimension $d_n$ and eigenenergy $E_n(t), H(t)|n^{\beta_n}(t)\rangle = E_n(t)|n^{\beta_n}(t)\rangle$; and assume that $d_n$ does not change during the total time...
An arbitrary state at \( t = 0 \) can be written as \( |\Psi(0)(0)\rangle = \sum_n \sum_{g_n=0}^{d_n-1} b_n(0) U^n_{h_n g_n}(0)|n(0)\rangle \), where \( |b_n(0)|^2 \) gives the probability of the system being in eigenspace \( \mathcal{H}_n \) and \( |b_n(0)U^n_{h_n g_n}(0)|^2 \) the probability of measuring a specific eigenstate. A given initial condition within an eigenspace is characterized by one value of \( h_n = 0, 1, \ldots, d_n - 1 \). A compact way of representing all possible initial conditions spanning the orthonormal eigenspace \( \mathcal{H}_n \) is \( |n(0)\rangle \), where \( |n(t)\rangle = (|n^0(t)\rangle, |n^1(t)\rangle, \ldots, |n^{d_n-1}(t)\rangle \) is a column vector, and \( U^n(0) \) a \( d_n \times d_n \) unitary matrix, \( U^n(0)U^n(0)\rangle = 1 \). A particular initial state corresponds to choosing the corresponding element of the column vector \( |\Psi(0)(0)\rangle \).

Then, the most general way of writing DAA is

\[
|\Psi(0)(t)\rangle = \sum_{n=0}^{\infty} e^{-i\omega_n(t)\delta_{n0}} B_n(0) U^n(t)|n(t)\rangle,
\]

where \( \omega_n(t) = \int_0^t E_n(t')dt' / h \) is the dynamical phase, and the unitary matrix \( U^n(t) = U^n(0)T \exp(i\int_0^t A^n(t')dt') \) the non-Abelian Wilczek-Zee phase (WZ phase). Here \( T \) denotes a time-ordered operator, and \( A^{nm}(t) = (M^{nm})_h g_n(t) \) a \( d_n \times d_n \) matrix defined as

\[
[M^{nm}(t)]_{g_n h_m} = M^{nm}(h_m g_n(t)) = \langle n^g(t)|m^n(0)\rangle,
\]

with the dot meaning time derivative. For example, for a system starting at the ground eigenspace \( (b_n(0) = \delta_{n0}) \),

\[
|\Psi(0)(t)\rangle = e^{-i\omega_0(t)} U^0(t)|0(0)\rangle.
\]

The time evolution of an informationally isolated quantum system is dictated by the Schrödinger equation (SE) \( i\hbar |\dot{\Psi}(t)\rangle = H(t)|\Psi(t)\rangle \). What are the constraints on the rate of change of \( H(t) \) under which the system’s evolved state \( |\Psi(t)\rangle \) gets close to DAA? The adiabatic theorem we formulate next sets the conditions under which DAA holds. In other words, it precisely states when the system's dynamics can be approximated by DAA.

**Adiabatic Theorem:** If a system’s Hamiltonian \( H(t) \) changes slowly during the course of time, say from \( t = 0 \) to \( T \), and the system is prepared in an arbitrary superposition of eigenstates of \( H(t) \) at \( t = 0 \), say \( |\Psi(0)(0)\rangle \), then the transitions between eigenspaces \( \mathcal{H}_n \) of \( H(t) \) during the interval \( t \in [0, T] \) are negligible and the system evolves according to DAA.

The three important concepts, slow, negligible, and evolved state, need further explanation. First, DAA is based on the assumption that the rate of change of \( H(t) \) is slow. A crucial matter is then to establish the meaning of slow precisely. Intuitively, the latter notion can be understood as a relation between a characteristic internal time of the evolved system \( T_e \), encoded in \( H(t) \), and the total evolution time \( T \), such that \( T_e / T \ll 1 \). For a fixed and finite \( T_e \), one can always choose an evolution time \( T \) that satisfies this condition. This state of affairs, however, is not satisfactory from a mathematical standpoint. Indeed, a main source of controversy in the literature arises from the lack of a precise quantification of the term slow. By using the degenerate adiabatic perturbation theory (DAPT) \( 8 \), a generalization of APT \( 8 \), we can give a precise meaning to this notion of slowness, which is the key ingredient to the derivation of the sufficient condition of DAT. Second, to establish the necessary condition we follow Tong \( 8 \) and others \( 10–12 \) and assume that if the system’s state is well described by DAA then all measurements performed on the system at any time must indeed be consistent with this assumption. This has a profound implication on the approximate dynamics the system obeys \( 8 \). The following necessary and sufficient conditions provide the mathematical rigor required to make those concepts precise.

**The necessary condition.** There is no unique way of establishing how close two quantum states are, implying that there is no unique distance measure between states. A popular choice in the context of quantum information is the fidelity measure. We stress though that DAT is not a statement about the fidelity between the true time-dependent state \( |\Psi(t)\rangle \) and DAA \( |\Psi(0)(t)\rangle \) being close to one, i.e., \( |||\Psi(t)|\Psi(0)(t)|| \approx 1 \). It is more than that, it is a statement about DAA expectation value of any observable being close to the exact ones. This notion is crucial to define geometric phases, thus for particle exchange statistics, and is crucial for the philosophy behind DAPT and the proof of necessity that now follows.

If DAA is an accurate description of the time evolution of a degenerate system starting, with no loss of generality, in its ground eigenspace \( (b_n(0) = \delta_{n0}) \) then \( |\Psi(t)\rangle = |\Psi(0)(t)\rangle + O(1/T) \approx |\Psi(0)(t)\rangle \), with \( |||O(1/T)|| \max \ll 1 \), where \( |||\cdot||| \max \) is the max norm (the absolute value of the greatest element of a given vector/ matrix). It immediately follows that the system (a) approximately satisfies SE \( i\hbar |\dot{\Psi}(0)(t)\rangle \approx H(t)|\Psi(0)(t)\rangle \) which implies \( 8 \) that (b) transitions to excited eigenspaces are negligible \( 13 \), \( \frac{|||\langle n(t)|\Psi(t)\rangle^2||| \max \approx 1, n \neq 0 \).

Now, using (a), (b), and defining \( \Delta_{nm}(t) = E_n(t) - E_m(t) \) we notice that for \( n \neq 0 \) \( 14 \),

\[
(n(t)|^T|\Psi(t)\rangle)^T = \frac{\langle n(t)|^T(H(t) - E_0(t))|\Psi(t)\rangle^T}{\Delta_{n0}(t)}
\]

\[
\approx \frac{\langle n(t)|^T(\hbar h |\dot{\Psi}(t)\rangle - E_0(t)|\Psi(t)\rangle)^T}{\Delta_{n0}(t)}
\]

\[
\approx \frac{\hbar h |n(t)|^T |\dot{\Psi}(0)(t)\rangle^T}{\Delta_{n0}(t)}
\]

\[
= \hbar e^{-i\omega_n(t)} \frac{|n(t)|^T |U^n(t)|0(t)\rangle |^T \Delta_{n0}(t)}{\Delta_{n0}(t)}.
\]

where \( |n(t)|^T |0(t)\rangle |^T = 0 \). Taking the max norm on both sides and using (b) we get the necessary condition

\[
\hbar |||\langle n(t)|^T |U^n(t)|0(t)\rangle |^T \Delta_{n0}(t) || \max \ll 1, n \neq 0, t \in [0, T].
\]

Finally, using that \( |||U^n(t)|| \max \leq 1 \) leads to a
The zeroth order is exactly DAA, with WZ phase-free necessary condition,

$$h \left| \frac{\mathbf{M}^{(0)}(t)}{\Delta_{\text{n}}(t)} \right| \ll 1, \quad n \neq 0, \quad t \in [0, T],$$  

(3)

where \( \| A \|_1 = \max_{1 \leq i \leq p} \sum_{j=1}^{q} |a_{ij}| \) for a \( p \times q \) dimensional matrix \( A \). When the spectrum is non-degenerate (\( d_n = 1 \)), Eq. (3) reduces to the necessary condition of Ref. [2].

The sufficient condition. The first step to establish the sufficient condition is to prove the convergence of DAPT in its full generality. Intrinsic to the formulation of DAPT is a Taylor series expansion in terms of the parameter \( v = 1/T \), and a necessary rescaling of time according to \( s = vt \) with \( s \in [0, 1] \) [2]. For small enough \( v \) one can always make DAPT converge (cf. Eq. (3)).

Inserting the ansatz

$$|\Psi(s)\rangle = \sum_{n=0}^{\infty} \sum_{p=0}^{\infty} C^{(p)}_{n}(s)|n(s)\rangle$$  

(4)

into SE with \( C^{(p)}_{n}(s) = e^{-\frac{i}{\hbar} \omega_n(s)} v^p B^{(p)}_{n}(s) \) and \( B^{(p)}_{n}(s) = \sum_{m=0}^{\infty} e^{\frac{i}{\hbar} \omega_m(s)} B^{(p)}_{m}(s) \), DAPT gives recursive equations for \( B^{(p)}_{m}(s) \) in terms of lower order in \( p \) coefficients [3]. The zeroth order is exactly DAA, with WZ phase-naturally appearing as a requirement for the consistency of the series expansion. Note that for each \( n \) we have a series involving the matrix \( C^{(p)}_{n}(s) \), \( p = 0, 1, \ldots, \infty \). The matrix element \( C^{(p)}_{n}(s) \) handles the coefficient giving the contribution to order \( p \) of the state \( |\eta^{(n)}(s)\rangle \) to the solution to SE. Here \( h_n \) handles different initial conditions and for definiteness we pick the case \( h_n = 0 \), \( \forall n \). Applying the ratio test for series expansions, if the condition

$$\lim_{p \to \infty} \left| C^{(p+1)}_{n}(s)|_{0g_n} / C^{(p)}_{n}(s)|_{0g_n} \right| \ll 1, \quad \forall n, g_n,$$  

(5)

is satisfied for all coefficients then we guarantee convergence of DAPT. We can simplify further [4] by invoking the comparison test [14],

$$\lim_{p \to \infty} \sum_{m=0}^{\infty} \left| B^{(p+1)}_{m}(s)|_{0g_n} / B^{(p)}_{m}(s)|_{0g_n} \right| < 1, \quad \forall n, g_n.$$  

(6)

Imposing that \( \sum_{p=0}^{\infty} |C^{(p+1)}_{n}(s)|_{0g_n} \ll |C^{(0)}_{n}(s)|_{0g_n} \), \( \forall n, g_n \), meaning that the zeroth order dominates, is equivalent to

$$\sum_{p=0}^{\infty} \sum_{m=0}^{\infty} v^{p+1} \left| B^{(p+1)}_{m}(s)|_{0g_n} \right| \ll \sum_{m=0}^{\infty} \left| B^{(0)}_{m}(s)|_{0g_n} \right|,$$  

(7)

which together with Eq. (3) are the rigorous sufficient conditions for the validity of DAA. In practice it is extremely difficult to compute the previous limit when \( p \to \infty \) and all orders \( p \). We can come up, nevertheless, with some practical condition of convergence by looking at the ratio for a couple of finite orders \( p \). Working with increasing \( p \) we get more and more conditions that, in the non-degenerate case, can become stronger than the ones in [12]. In its simplest form, we may consider only \( p = 0 \). In this case both expressions merge into one and we demand it to be much smaller than the smallest non-null term appearing in the rhs of (7). Thus, the practical sufficient test reads

$$v \sum_{m=0}^{\infty} \left| B^{(1)}_{m}(s)|_{0g_n} \right| \ll \min_{n-g_0} \sum_{m=0}^{\infty} \left| B^{(0)}_{m}(s)|_{0g_n} \right|.$$  

(8)

Using [3] \( B^{(0)}_{m}(s) = b_n(0) U^n(s) \delta_{mn} \) and the fact that at \( t = 0 \) the initial state is \( |\eta^{(0)}(0)\rangle \) (\( b_n(0) = \delta_{na} \)) we get

$$v \sum_{m=0}^{\infty} \left| B^{(1)}_{m}(s)|_{0g_n} \right| \ll \min_{n_0} \left( \left| U^{(0)}(s)|_{0g_n} \right| , \forall n, g_n,$$  

(9)

which is our intuitive and practical sufficient condition. Indeed, noting that \( v \sum_{m=0}^{\infty} e^{-\frac{i}{\hbar} \omega_m(s)} B^{(1)}_{m}(s)|_{0g_n} \), with \( n \neq 0 \), gives the first order contribution of the excited state \( |\eta^{(n)}(s)\rangle \) to the wave equation, and that for \( n = 0 \) it is related to the first order correction to the WZ phase [3], it is clear that they must be much smaller than the smallest coefficient appearing in the zeroth order if we want DAA to hold.

Equation (9) also depends on \( U^n(s) \) because \( B^{(1)}_{m}(s) \) depends on \( U^n(s) \). However, a similar calculation to the one done for the necessary condition gets rid of these unitary matrices leading to [14]

$$D^{(n)}_{g_0}(t) \ll \min_{g_0} \left( \left| U^{(0)}(s)|_{0g_0} \right| , \quad t \in [0, T],$$  

(10)

where for \( n = 0 \) and \( \forall g_0 \) we have \( D^{(0)}_{g_0}(t) \) equals to

$$h d_0 \int dt' \sum_{n=1}^{d_0-1} \frac{\sum_{k_0}^{d_0-1} \left| \mathbf{M}^{(n)}(t')|\mathbf{M}^{(n)}(t')\right|_{k_0,l_0}}{\left| \Delta_{\text{g}_0}(t') \right|},$$  

(11)

and for \( n \neq 0 \) and \( \forall g_n \), \( D^{(n)}_{g_n}(t) \) is given by

$$\frac{h}{\left| \Delta_{\text{g}_0}(0) \right|} \sum_{k_{0}}^{d_0-1} \sum_{l_{0}}^{d_0-1} \left| \mathbf{M}^{(n)}(t)|_{k_{0}g_0} + d_n \sum_{k_{0},l_{0}} \left| \mathbf{M}^{(0)}(t)|_{k_0,l_0} \right| \right|.$$  

(12)

Example. We now apply the previous ideas to a doubly degenerate four-level system subject to a rotating magnetic field of constant magnitude \( B(t) = Br(t) \) and in spherical coordinates \( r(t) = (\sin \theta \cos w t, \sin \theta \sin w t, \cos \theta) \), with \( w > 0 \) and \( 0 < \theta \leq \pi \) being the polar angle. The Hamiltonian describing this system is [3, 13] \( \mathbf{H}(t) = h B r(t) \cdot \Gamma / 2 \), where \( b > 0 \) is proportional to the coupling between the field and the system and \( \Gamma = (\Gamma_x, \Gamma_y, \Gamma_z) \) are the Dirac matrices \( \Gamma_j = \sigma_x \otimes \sigma_j, \quad j = x, y, z \). Here \( \sigma_j \) are the standard Pauli matrices imposing the following
algebra for $\Gamma_j$, \{\Gamma_i, \Gamma_j\} = 2\delta_{ij}I_4$, \{\Gamma_i, I_j\} = 2\epsilon_{ijk}\Pi_k$, where $I_4$ is the identity matrix of dimension four, $\delta_{ij}$ the Kronecker delta, $\epsilon_{ijk}$ the Levi-Civita symbol, and $\Pi_k = I_2 \otimes \sigma_k$. Starting at the ground state $|00(0)\rangle$ the time-dependent solution in terms of the snapshot eigenstates is $|\Psi(t)\rangle = e^{iwt/2} |1 + \cos \theta \rangle A_-(t) + (1 - \cos \theta) A_-(t)/(2 |0\rangle + e^{-iwt/2} \sin \theta (A_+(t) - A_-(t))/2 |0\rangle + e^{iwt/2} \sin^2 \theta (B_+(t) + B_-(t))/2 |1\rangle(t) + e^{-iwt/2} \sin \theta (|1\rangle + \cos \theta) B_-(t) - (1 - \cos \theta) B_+(t))/2 |1\rangle(t)$, where $A_\pm(t) = \cos(\Omega t/2) + i (\pm 2 w \cos \theta) / \Omega \pm i \sin(\Omega t/2) / \Omega$, $B_\pm(t) = i w \sin(\Omega t/2) / \Omega$, $\Omega^2 = \omega^2 + 2b^2 \pm 2wb \cos \theta$.

Necessary condition. Since in this example Eq. (2) is $|M^{10}(t)\rangle_{11} = -|M^{10}(t)\rangle_{00} = iw \sin^2 \theta / 2$ and $|M^{10}(t)\rangle_{10} = -|M^{10}(t)\rangle_{01} = -iw \sin(2\theta) e^{iwt/4}$ the necessary condition (3) becomes $w\sin \theta \sin \theta + \cos \theta (b/2b) < 1$. Our task now is to look at the exact solution, impose that DAA holds, and see if it implies the necessary condition above. If DAA holds then the absolute values of the coefficients multiplying $|10\rangle(t)$ and $|11\rangle(t)$ of the exact solution are negligible. Working with the largest of those this is equivalent to showing that $|wg(\theta)/b - 1| < 1$, with $g(\theta) = \sin \theta / (b + \Omega - b/\Omega)$. Using that $g(\theta)$ has a maximum of $\pi/2$ for $\theta \in [0, \pi]$, at $\theta = \pi/2$ given by $2b/(b^2 + w^2)$ we get $wg(\theta)/b \leq 2b/(b^2 + w^2)^{1/2} \leq 2b/b$. Hence, if the sufficient conditions imply that $2b/b < 1$ we are done. But noting that $|\sin(wt \cos \theta)/2|/(\cos \theta + \sin \theta) < 1/2$ the sufficient conditions reduce to $5w/2b < 1$ which obviously implies $2w/b < 1$.

Summary. We established one rigorous necessary condition and two sufficient conditions, one rigorous and one practical, for the validity of the quantum adiabatic theorem for systems with degenerate spectra. Concepts such as “slowly/adiabatically changing Hamiltonians” and the “adiabatic approximation” for degenerate systems, of greatest importance for the implementation of adiabatic and topological quantum computation as well as non-Abelian fractional statistics, were quantitatively stated. It is this quantitative specification that allows for a precise and rigorous formulation of the adiabatic theorem. Finally, we applied the adiabatic theorem to an exactly solvable degenerate problem, and provided a complete characterization of the mathematical conditions under which the degenerate adiabatic approximation holds.

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Note that when $t \approx 0$ and/or $\theta \approx \pi/2$, $|U^0(t)_{01}| \approx 0$ and we must work with the non-null coefficient $|U^0(t)_{00}|$. In this case the sufficient condition is $5w/(2b) \ll 1$.

It is important to remark now that if $w \geq b$ we cannot satisfy the sufficient condition, no matter what the value of $\sin \theta$ is. Indeed, since both terms appearing at the rhs of the sufficient conditions are smaller than one, assuming $w \geq b$ leads to a lhs greater than one. The sufficient conditions are then consistent with the cases where the necessary condition fails. We cannot have $\sin \theta \approx 0$ and $w \geq b$ as an instance in which the necessary condition fails.
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