Adiabatic Approximation

The reaction of a system to a time-dependent perturbation depends in detail on the time scale of the perturbation.

Consider, for example, an ideal pendulum, with no friction or air resistance, oscillating back and forth in a vertical plane. If we move the support ‘quickly’, the motion of the bob will be wildly chaotic. On the other hand, if we move the support ‘gradually’, the bob will continue to oscillate smoothly, in the same plane (or one parallel to it) and with the same amplitude.

This gradual change in the external conditions characterizes an adiabatic process. The quick movement which had a chaotic effect is often referred to as sudden.

Note that the term ‘adiabatic’ does not imply anything with regard to the conservation of the energy of the system.

Not surprisingly, quantum systems are affected in ways analogous to this classical system.
First, we must get more quantitative regarding the qualitative phrases ‘quickly’ and ‘gradually’.

Considering the case of the pendulum in more detail, there is clearly a time scale associated with any movement of the support which is appreciable on the scale of its oscillation amplitude, $T_e$. Similarly, $T_i$ is related to the oscillation period of the bob. An adiabatic process is one for which $T_e \gg T_i$.

Note that the overall scale of the total change in position is not important, and could be very large.

The basic strategy for analyzing an adiabatic process is to first solve for the behavior of the system with the external parameters held fixed. Then, at the end of the calculation, allow them to change.
For example, the classical period of a pendulum of constant length $L$ is $2\pi\sqrt{L/g}$. If the length is now changing ‘gradually’ (adiabatically), then the period is presumably $2\pi\sqrt{L(t)/g}$.

We have used this approach already. For example, the frequency of vibration of the nuclei of the hydrogen molecule was obtained by assuming a separation $R$, solving the electron eigenstate problem for fixed nuclei, determining which $R$ yields the lowest total energy, and calculating the net nucleus-nucleus force (problem 7.10). In molecular and solid state physics, this differential treatment of electron and nuclear motions is called the ‘Born-Oppenheimer approximation’.
Adiabatic theorem

Figure - A model for adiabatic change of the Hamiltonian, from $H^i$ to $H^f$.

Suppose that the Hamiltonian changes ‘gradually’ from $H^i$ to $H^f$. If the particle is initially in the $n^{\text{th}}$ eigenstate of $H^i$, it will be carried (under the Schrödinger equation) into the $n^{\text{th}}$ eigenstate of $H^f$.

It is assumed that the spectrum is discrete, and nondegenerate throughout the transition from $H^i$ to $H^f$, so that there is no ambiguity about the ordering of the eigenstates.
For example, consider a particle in the ground state of the infinite square well: 
\[ \psi_0^i(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right). \]

If we move the wall gradually out to \(2a\), the adiabatic theorem predicts that the particle will end up in the ground state of the expanded well: 
\[ \psi_0^f(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{\pi}{2a}x\right). \]

On the other hand, if we move the wall ‘suddenly’, the particle position cannot respond on the time scale of the change. Thus the final state is a complicated sum over all of the eigenstates of \(H^f\): 
\[ \psi(x) = \sum \psi_n^{f}(x) \langle \psi_n^{f} | \psi_0^i \rangle. \]

Figure 10.2 - (a) Particle starts out in the ground state of the infinite square well. (b) If the wall moves slowly, the particle remains in the ground state. (c) If the wall moves rapidly, the particle is left (momentarily) in its initial state (which is not an eigenstate of the (new) Hamiltonian).
Since the proof of the adiabatic theorem is complicated, I will give you only a plausibility argument.

Consider a Hamiltonian which changes ‘gradually’ from $H^i$ to $H^f = H^i + V$ between $t = 0$ and $t = T$, and focus on a particle in the state $n$ at $t = 0$ (i.e., $\Psi(0) = \psi^i_n$).

Figure - A model for an adiabatic transition, where $H'(t) = Vf(t)$. 

\[ f(t) \]
If $V$ is small enough that we can use time-dependent perturbation theory, the overlap of the final-state w.f. with the e.s.’s of $H^f$ is $|\langle \Psi(T) | \psi_m^f \rangle|^2 = \delta_{nm} + O(V^2)$. In other words, the probability of inducing a transition is $O(V^2)$.

If $V$ is not small, we divide $V$ into $N$ steps of $\frac{V}{N}$. This yields a total transition probability of order $< N(\frac{V}{N})^2 = \frac{V^2}{N} \to 0$ as $N \to \infty$. ‘QED’
Consider again the portable pendulum. Suppose we place it at the North Pole and set it oscillating in the plane which includes Troy. Ignoring for the moment the rotation of the earth, let’s move the pendulum adiabatically south along the intersection of that plane with the earth to the equator, for example, then west along the equator for, say, 30°, and then north along that longitude line to the North Pole. At all times, the pendulum has oscillated in a plane oriented ‘north–south’. Yet now that plane makes an angle of 30° with the original plane of oscillation.

Figure 10.5 - A path for adiabatic transport of a pendulum on the surface of the earth.
The axis of oscillation has been rotated by \( \Theta = 30^\circ \) about a perpendicular axis (i.e., the earth's axis). A moment's reflection suggests that this rotation occurred during the movement along the equator. Furthermore, analysis shows that the amount of the rotation is equal to the solid angle subtended at the center of the earth by the path on the surface: \( \Theta \equiv \Omega \).

Figure 10.6 - Arbitrary path on the surface of a sphere, subtending a solid angle \( \Omega \).

The action of a Foucault pendulum can be explained in the same way, differing only in that the earth's rotation is the mechanism for the pendulum tracing the path.
A system such as this, which does not return to its original state when transported around a closed loop, is said to be *nonholonomic*. [Note that the ‘transport’ need not be physical.]

In the context of quantum mechanics, we will be concerned with situations in which external parameters are altered in some way, and then returned to their initial values, all adiabatically.
It is important to understand exactly what we mean by the adiabatic theorem. In particular, the statement that the system remains in its ‘original state’ throughout an adiabatic process does not preclude a change in phase. [In general in quantum mechanics, there is a certain arbitrariness regarding phase.]

Even in the case of a time independent Hamiltonian, a particle in the \( n^{th} \) e.s. will undergo a steady progression of its phase:
\[
\Psi_n(x, t) = \psi_n(x)e^{-iE_n t/\hbar}.
\]

Generalizing this to the case of a Hamiltonian which changes with time,
\[
\Psi_n(x, t) = \psi_n(x, t)e^{-i \int_0^t dt' E_n(t')} e^{i \gamma_n(t)}.
\]

The factor containing the integral of \( E_n(t') \) over time generalizes the standard factor, \( e^{-iE_n t/\hbar} \) to the case where \( E_n \) is a function of time. This is known as the ‘dynamic phase’. Any extra phase, \( \gamma_n(t) \), is called the ‘geometric phase’. 

To determine the ‘geometric phase’, substitute the generalized equation for $\Psi_n(x,t)$ into the time-dependent Schrödinger equation:
\[ \frac{d\gamma_n}{dt} = i\langle \psi_n | \frac{\partial \psi_n}{\partial t} \rangle. \]
$\gamma_n(t)$ is obtained by integrating this equation over $t$.

The phase $\gamma_n(t)$ is determined by some set of parameters in the Hamiltonian which are changing as a function of time, $R_1(t), R_2(t), \cdots \Rightarrow \mathbf{R}(t)$. Assuming that all of these parameters return to their original values after some interval $T$, we can substitute an integral over these parameters for the one over $t$:
\[ \gamma_n(T) = i \int d\mathbf{R} \cdot \langle \psi_n | \nabla_R \psi_n \rangle. \]
This is called ‘Berry’s phase’.
Several points can be made with regard to $\gamma_n$:

1) $\gamma_n(t)$ is real, and can be shown to vanish if the $\psi_n$ can be defined as real.

2) Berry’s phase *is* measurable since it represents a *change* in the phase. Simply split a particle beam into two parts, put one through an adiabatically-changing potential, and combine the beams. The resultant phase change in one beam (only) will produce measurable interference.

3) The assumption of adiabaticity is *required* for the derivation.
Aharonov-Bohm effect

In classical electrodynamics, the potentials $\phi$ and $A$ are not directly measurable, only the resultant fields: $E = -\nabla \phi - \frac{\partial A}{\partial t}$, $B = \nabla \times A$.

In quantum mechanics, the potentials play a more fundamental role:

$$H = \frac{1}{2m} \left( \frac{\hbar}{i} \nabla - qA \right)^2 + q\phi.$$

In 1959 Aharonov and Bohm showed that electrons can be affected traveling through a region where $E$ and $B$ vanish but $A$ does not, *completely contrary* to classical expectations.
They proposed an experiment in which a beam of electrons is split in two, the sub-beams pass on either side of an ideal solenoid, and are combined afterwards. The beams are kept well away from the solenoid to avoid any $B$ field (which is confined to the interior of the solenoid with only fringe fields outside). Nonetheless, the two beams are observed to arrive with phases which differ by $\frac{q\Phi}{\hbar}$, where $\Phi$ is the magnetic flux through the solenoid.

Figure 10.11 - Aharonov-Bohm effect: electron beam splits, with half passing on either side of a long solenoid.
In contrast with the behavior of $\mathbf{B}$ outside the solenoid, $\mathbf{A}$ declines only slowly with distance from the solenoid: $\mathbf{A} = \frac{\Phi}{2\pi r} \hat{\phi}$.

Putting $\mathbf{A}$ into $\mathbf{H}$, one can show that the spatial dependence of $\mathbf{A}$ leads directly to the following result for Berry’s phase:

$$\gamma_n(T) = \frac{q}{\hbar} \oint d\mathbf{R} \cdot \mathbf{A}(\mathbf{R}) = \frac{q}{\hbar} \int da \cdot (\nabla \times \mathbf{A}) = \frac{q\Phi}{\hbar},$$

where $\mathbf{R}$ is now a spatial variable.

This result agrees with the experimental result, and shows that the Aharonov-Bohm effect is a particular instance of geometric phase.