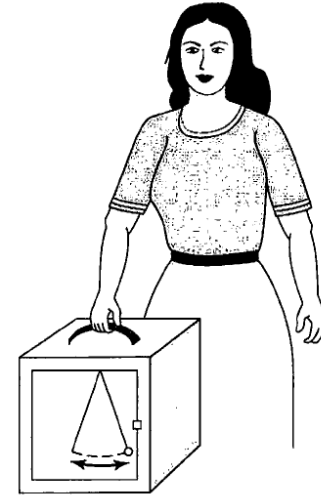


Section 11.5: The Adiabatic Approximation

Classical analog: a pendulum with zero friction oscillating in a plane. If abruptly you shake the box, the pendulum will have a complicated motion.

But if you "very slowly" rotate the box, the plane of oscillation will slowly rotate as well.

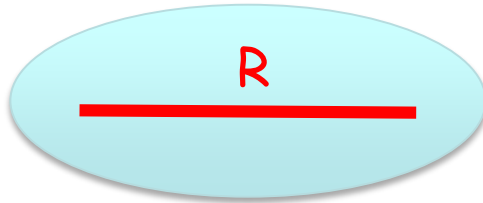


A very slow change in the boundary conditions of a problem defines an "adiabatic" process.

Often there are two characteristic times competing. One is internal, T_i , like the period of the pendulum that depends on gravity "g" and length of string "L". The other one is external, T_e , related in this example to the speed of rotation of the box. Adiabatic means $T_e \gg T_i$.

In QM this is often used in describing **oscillations of molecules**. Like we did for the H_2^+ ion: we fixed R the distance between hydrogens and solved the electron problem. The results depend on R of course. Then, by making $R=R(t)$ we could have found **the frequencies of oscillations of the atoms**, precursor of finding "phonons" in crystals.

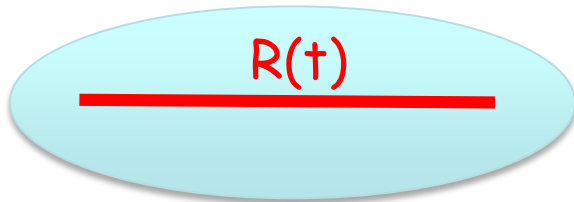
$$\psi = A [\psi_0(r_1) + \psi_0(r_2)] \text{ at } R \text{ fixed}$$



Same type of wave function

$$\psi = A [\psi_0(r_1) + \psi_0(r_2)]$$

simply at new $R(t)$

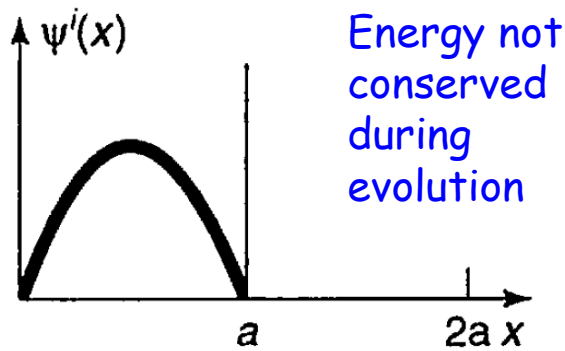


Solving the electronic problem first, and then addressing the oscillations in a fixed electronic cloud is called the **Born-Oppenheimer approximation**.

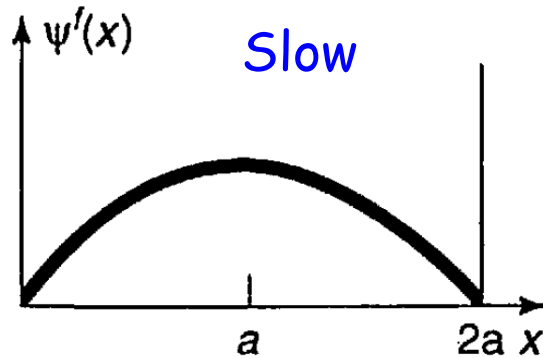
More specifically, if the electron was initially in the ground state, it remains in the ground state that smoothly changes its shape as R changes slowly. **This uses the Adiabatic Approximation !**

In general: if the particle is initially at eigenstate n th of initial H , then in an adiabatic problem it remains in the eigenstate n th of the final H .

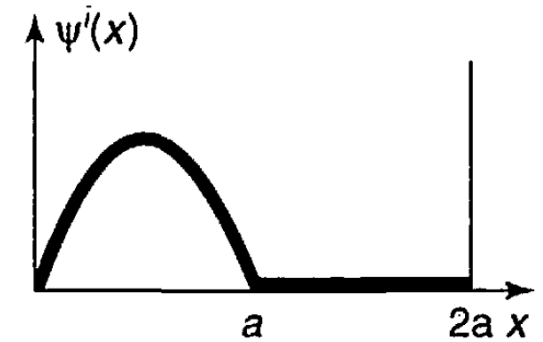
Now consider an **abrupt** switch from a to $2a$.



$$\psi^i(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right)$$



$$\psi^f(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{\pi}{2a}x\right)$$



The initial wave function is neither even nor odd, thus it will have a nonzero overlap with all the eigenstates!

Moreover, after the wall abruptly is moved to $2a$, the energy is **conserved** in the new problem. The electron will never be 100% in the ground state.

Definitely the wave function $\psi(t)$ will NOT be

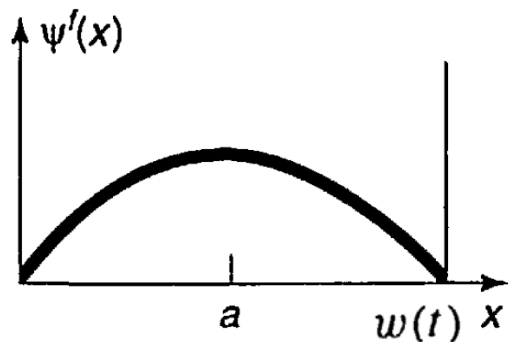
$$\psi^f(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{\pi}{2a}x\right)$$

The adiabatic theorem is complicated to prove. Specifically it says that in an adiabatic process the eigenstates -- assumed discrete energy spectrum so that you can follow each one -- evolve as:

$$\Psi_n(t) = e^{i\theta_n(t)} e^{i\gamma_n(t)} \psi_n(t)$$

For example, consider the square well again, with a wall moving with constant velocity v .

$$w(t) \equiv a + vt$$



$$\psi_n(x, t) = \sqrt{\frac{2}{w}} \sin\left(\frac{n\pi}{w}x\right)$$

In addition, there are two phase factors, according to the theorem: the dynamical and the geometrical (related to the Berry phase).

11.5.2: Start of proof of Adiabatic Theorem

First a reminder about the case H time independent.

$$H \psi_n = E_n \psi_n$$

$$\Psi_n(t) = \psi_n e^{-i E_n t / \hbar}$$

Even with a time independent Hamiltonian, for example a well with fixed "a", the wave functions pick up a phase as time t grows

A "unnecessarily complicated" way to write this phase is:

$$\theta_n(t) = -\frac{1}{\hbar} \int_0^t E_n(t') dt' = -\frac{1}{\hbar} E_n t$$

Consider now a **time dependent Hamiltonian**. At each instant of time " t " we can in principle solve the problem, but the eigenfunctions are different for each time " t ".

$$H(t) \psi_n(t) = E_n(t) \psi_n(t)$$

$$\langle \psi_n(t) | \psi_m(t) \rangle = \delta_{nm}$$

As explained in QM 411, at each instant of time "t" the time dependent Sch Eq is satisfied using a linear combination with properly chosen coefficients that now depend on time:

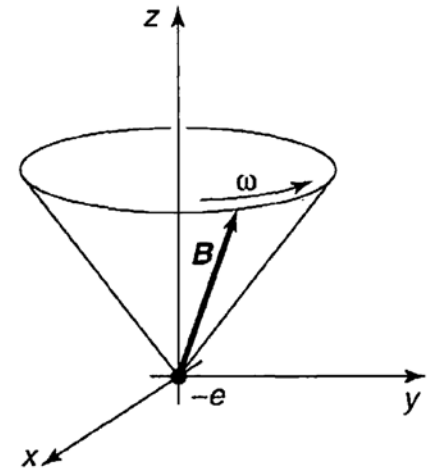
$$i\hbar \frac{\partial}{\partial t} \Psi(t) = H(t) \Psi(t) \quad \Psi(t) = \sum_n c_n(t) \psi_n(t) e^{i\theta_n(t)}$$

where the standard "dynamic phase" simply "accumulates" between different times:

$$\theta_n(t) = -\frac{1}{\hbar} \int_0^t E_n(t') dt'$$

But there is a second phase (explained in Griffiths second edition **but not in third**): the "geometric phase" already mentioned. Differences of this geometrical phase are the Berry phase much discussed in condensed matter physics at present.

Example 11.4. Consider an electron static at origin of coordinates in a magnetic field with constant magnitude B_0 but with direction rotating forming a **cone**, at **angular velocity ω and angle α** :



$$\mathbf{B}(t) = B_0[\sin \alpha \cos(\omega t)\hat{i} + \sin \alpha \sin(\omega t)\hat{j} + \cos \alpha \hat{k}]$$

The Hamiltonian is a 2x2 matrix involving the Pauli matrices:

$$\begin{aligned} H(t) &= \frac{e}{m} \mathbf{B} \cdot \mathbf{S} = \frac{e\hbar B_0}{2m} [\sin \alpha \cos(\omega t)\sigma_x + \sin \alpha \sin(\omega t)\sigma_y + \cos \alpha \sigma_z] \\ &= \frac{\hbar\omega_1}{2} \begin{pmatrix} \cos \alpha & e^{-i\omega t} \sin \alpha \\ e^{i\omega t} \sin \alpha & -\cos \alpha \end{pmatrix} \quad \text{with} \quad \omega_1 \equiv \frac{eB_0}{m} \end{aligned}$$

This problem can be solved exactly, being just a 2x2 matrix. The eigenspinors and energies are:

$$\chi_+(t) = \begin{pmatrix} \cos(\alpha/2) \\ e^{i\omega t} \sin(\alpha/2) \end{pmatrix} \quad \chi_-(t) = \begin{pmatrix} e^{-i\omega t} \sin(\alpha/2) \\ -\cos(\alpha/2) \end{pmatrix} \quad E_{\pm} = \pm \frac{\hbar\omega_1}{2}$$

$$\omega_1 \equiv \frac{eB_0}{m}$$

IMPORTANT: these are solutions at a fixed time t , and **they represent spin up and down along the instantaneous direction of \mathbf{B} which is changing orientation with time.**

Suppose the electron starts "up" along the direction of the field \mathbf{B} at time $t=0$

$$\chi(0) = \begin{pmatrix} \cos(\alpha/2) \\ \sin(\alpha/2) \end{pmatrix}$$

The question is: can the electron follow the magnetic field as it rotates in the cone, keeping the "up" orientation?

This problem can be solved exactly at any arbitrary time "t".
It can be shown that the following spinor is the solution:

$$\chi(t) = \begin{pmatrix} \left[\cos(\lambda t/2) - i \frac{(\omega_1 - \omega)}{\lambda} \sin(\lambda t/2) \right] \cos(\alpha/2) e^{-i\omega t/2} \\ \left[\cos(\lambda t/2) - i \frac{(\omega_1 + \omega)}{\lambda} \sin(\lambda t/2) \right] \sin(\alpha/2) e^{+i\omega t/2} \end{pmatrix}$$

$$\lambda \equiv \sqrt{\omega^2 + \omega_1^2 - 2\omega\omega_1 \cos \alpha}$$

Expressed in terms of the up and down basis (you will do it in HW10) along the **B** direction:

$$\begin{aligned} \chi(t) = & \left[\cos\left(\frac{\lambda t}{2}\right) - i \frac{(\omega_1 - \omega \cos \alpha)}{\lambda} \sin\left(\frac{\lambda t}{2}\right) \right] e^{-i\omega t/2} \chi_+(t) \\ & + i \left[\frac{\omega}{\lambda} \sin \alpha \sin\left(\frac{\lambda t}{2}\right) \right] e^{+i\omega t/2} \chi_-(t). \end{aligned}$$

Then the projection of the exact result along the "up" and "down" instantaneous directions can be obtained (HW10). For "down" is:

$$|\langle \chi(t) | \chi_-(t) \rangle|^2 = \left[\frac{\omega}{\lambda} \sin \alpha \sin\left(\frac{\lambda t}{2}\right) \right]^2$$

This result is EXACT at any time and any rotation angular velocity.

Having an **exact solution** is ideal to study the **adiabatic approximation**!

It is important to identify the **external and internal characteristic times**:

$$T_e = 1/\omega$$

$$\mathbf{B}(t) = B_0[\sin \alpha \cos(\omega t)\hat{i} + \sin \alpha \sin(\omega t)\hat{j} + \cos \alpha \hat{k}]$$

$$T_i = \hbar/(E_+ - E_-) = 1/\omega_1$$

$$E_{\pm} = \pm \frac{\hbar\omega_1}{2} \quad \omega_1 \equiv \frac{eB_0}{m}$$

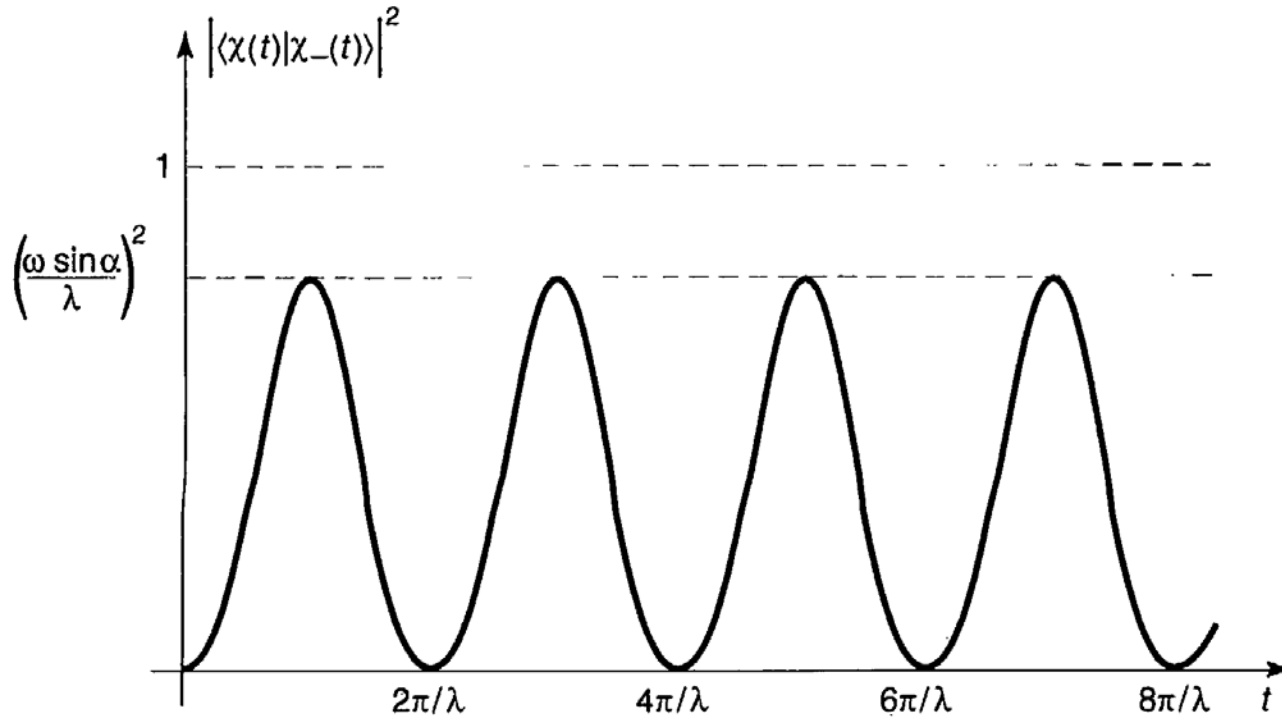
The adiabatic approximation is when $T_e \gg T_i$, namely $\omega \ll \omega_1$.

$$|\langle \chi(t) | \chi_-(t) \rangle|^2 = \left[\frac{\omega}{\lambda} \sin \alpha \sin \left(\frac{\lambda t}{2} \right) \right]^2 \cong \left[\frac{\omega}{\omega_1} \sin \alpha \sin \left(\frac{\lambda t}{2} \right) \right]^2 \rightarrow 0$$

If $\frac{\omega}{\omega_1} \rightarrow 0$ then $\lambda \equiv \sqrt{\omega^2 + \omega_1^2 - 2\omega\omega_1 \cos \alpha} \rightarrow \omega_1$

In the adiabatic limit the magnetic field leads the electron "by its nose" to rotate its orientation all the time pointing along $\mathbf{B}(t)$.

$$|\langle \chi(t) | \chi_{-}(t) \rangle|^2 = \left[\frac{\omega}{\lambda} \sin \alpha \sin \left(\frac{\lambda t}{2} \right) \right]^2$$



In exact solution, the probability of "down spin" will not be zero. It will oscillate. But weight is regulated by ω/λ . Thus, in adiabatic limit the amplitude will be minuscule.

The new edition of Griffiths does NOT explain the origin of the geometrical phase. Below, for those interested, is the proof from the second edition. **From here down, this portion is NOT part of the TEST 3.**

As explained in QM 411, at each instant of time "t" the time dependent Sch Eq is satisfied using a linear combination with properly chosen coefficients that now depend on time:

$$i\hbar \frac{\partial}{\partial t} \Psi(t) = H(t) \Psi(t) \quad \Psi(t) = \sum_n c_n(t) \psi_n(t) e^{i\theta_n(t)}$$

where the standard "dynamic phase" simply "accumulates" between different times:

$$\theta_n(t) = -\frac{1}{\hbar} \int_0^t E_n(t') dt'$$

But there is a second phase (explained in Griffiths second edition **but not in third**): the "geometric phase".

Placing $\Psi(t) = \sum c_n(t) \psi_n(t) e^{i\theta_n(t)}$ into $i\hbar \frac{\partial}{\partial t} \Psi(t) = H(t) \Psi(t)$ we obtain a diff eq for $c_n(t)$ like we did before for $c_a(t)$ and $c_b(t)$ studying emission:

$$i\hbar \sum_n [\dot{c}_n \psi_n + c_n \dot{\psi}_n + \cancel{i c_n \psi_n \dot{\theta}_n}] e^{i\theta_n} = \sum_n c_n (\cancel{H \psi_n}) e^{i\theta_n}$$

because

$$\frac{\partial}{\partial t} \theta_n(t) = -\frac{1}{\hbar} \frac{\partial}{\partial t} \int_0^t E_n(t') dt' = -\frac{1}{\hbar} E_n(t)$$

Then we simplified from four terms to just two:

$$\sum_n \dot{c}_n \psi_n e^{i\theta_n} = - \sum_n c_n \dot{\psi}_n e^{i\theta_n}$$

Consider the inner product with $\langle \psi_m |$ and use orthonormality at time t :

$$\sum_n \dot{c}_n \delta_{mn} e^{i\theta_n} = - \sum_n c_n \langle \psi_m | \dot{\psi}_n \rangle e^{i\theta_n}$$

Note time derivative

$$\dot{c}_m(t) = - \sum_n c_n \langle \psi_m | \dot{\psi}_n \rangle e^{i(\theta_n - \theta_m)}$$

The sum over n contains both $n=m$ and $n \neq m$.

$n \neq m$ can be neglected under the **adiabatic condition** as shown in next page (optional, read if interested, otherwise move to the following page).

OPTIONAL
PAGE

$$H(t)\psi_n(t) = E_n(t)\psi_n(t)$$

$$\dot{H}\psi_n + H\dot{\psi}_n = \dot{E}_n\psi_n + E_n\dot{\psi}_n$$

Again consider the inner product with $\langle\psi_m|$:

$$\langle\psi_m|\dot{H}|\psi_n\rangle + \langle\psi_m|H|\dot{\psi}_n\rangle = \dot{E}_n\delta_{mn} + E_n\langle\psi_m|\dot{\psi}_n\rangle$$

Use Hermiticity of H (that we learn in Ch 3) and assume $n \neq m$.

$$\langle\psi_m|H|\dot{\psi}_n\rangle = E_m\langle\psi_m|\dot{\psi}_n\rangle$$

$$\langle\psi_m|\dot{H}|\psi_n\rangle = (E_n - E_m)\langle\psi_m|\dot{\psi}_n\rangle$$

Only now we use the **adiabatic condition** and declare that this term has to be very small because it involves a time derivative of H .

Since $n \neq m$ then $\langle\psi_m|\dot{\psi}_n\rangle$ has to be \sim zero for $n \neq m$.

Then, using the proof in the previous page, in the equation two pages back we can drop all terms with $n \neq m$.

$$\dot{c}_m(t) = - \sum_n c_n \langle \psi_m | \dot{\psi}_n \rangle e^{i(\theta_n - \theta_m)} \longrightarrow \dot{c}_m(t) = -c_m \langle \psi_m | \dot{\psi}_m \rangle$$

solve

$$c_m(t) = c_m(0) e^{i\gamma_m(t)}$$

$$\gamma_m(t) \equiv i \int_0^t \left\langle \psi_m(t') \left| \frac{\partial}{\partial t'} \psi_m(t') \right. \right\rangle dt'$$

this phase factor is called the "geometric phase"

Assume electron is in state "n" at time $t=0$:

$$c_n(0) = 1 \quad c_m(0) = 0$$

The solution tells us that all coefficients with $n \neq m$ remain 0 while the coefficient "n" acquires a phase factor. Thus, overall the full wave function picks up a "dynamical phase" and a "geometrical phase":

$$\Psi_n(t) = e^{i\theta_n(t)} e^{i\gamma_n(t)} \psi_n(t)$$