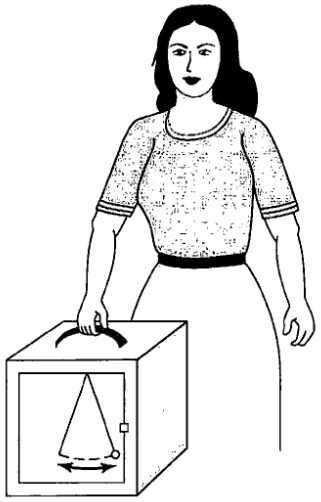
Chapter 10: The Adiabatic Approximation

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



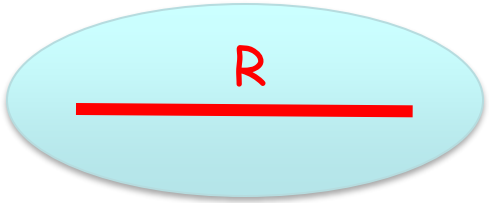
But if you "very slowly" rotate the box, the plane of oscillation will slowly rotate as well.

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 "g" and length of string "L". The other one is external, T_e, related in the example to the speed of rotation of the box.
Adiabatic means $T_e >> T_i$.

In QM this is often used in describing oscillations of molecules. Like we did for the H_2^+ ion, we fix R the distance between hydrogens and solve 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.

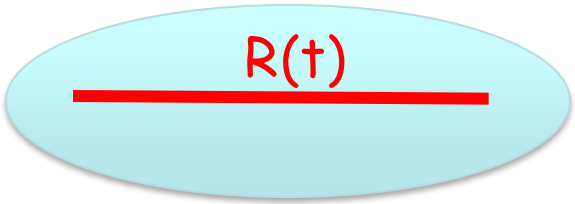
$\psi = A\,[\psi_0(r_1) + \psi_0(r_2)]$ at R fixed



Same type of wave function

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

simply at new R (t)

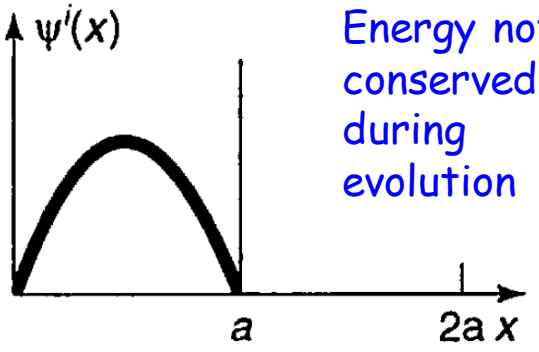


Solving the electronic problem first, and then addressing the oscillations in a fixed electronic cloud is called the **Born-Oppenheimer approximation**.

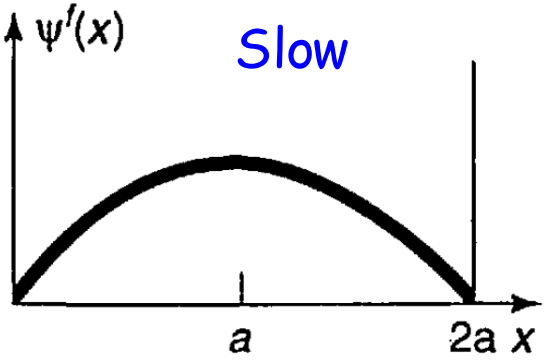
More specifically, if the electron was initially in the ground state, it remains in the ground state that smoothly changes its shape as R changes slowly.

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

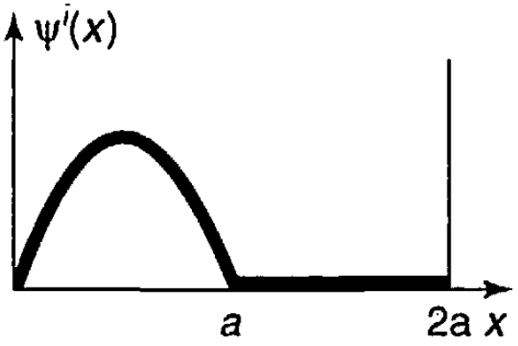
Now consider an **abrupt** switch from a to 2a.



Energy not conserved during evolution



Slow



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

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

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

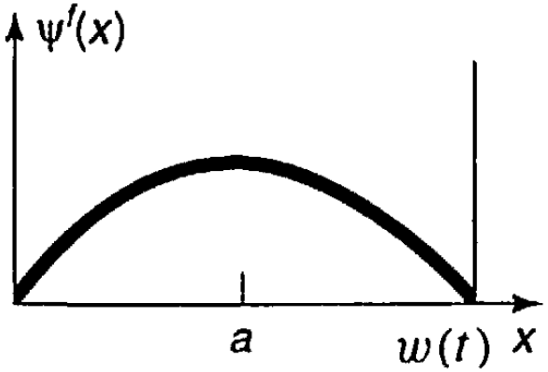
$$\psi^f(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{\pi}{2a}x\right)$$

The adiabatic theorem is complicated to prove but we will try. Specifically it says that in an adiabatic process the eigenstates -- assumed discrete 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.

10.1.2: Proof of the Adiabatic Theorem

First a reminder about the case H time independent.

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

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 "difficult" 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".

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

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

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

where the standard "dynamic phase" simply "accumulates" between different times: $\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\,dt'$

Placing $\Psi(t) = \sum_n c_n(t)\psi_n(t)e^{i\theta_n(t)}$ 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:

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

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

OPTIONAL

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

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

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

Then, in the equation two pages back we can drop all terms with n≠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

$$c_m(t) = c_m(0) e^{i\gamma_m(t)} \qquad \gamma_m(t) \equiv i \int_0^t \left\langle \psi_m(t') \left| \frac{\partial}{\partial t'} \psi_m(t') \right\rangle dt'$$

this phase factor
is called the "geometric phase"

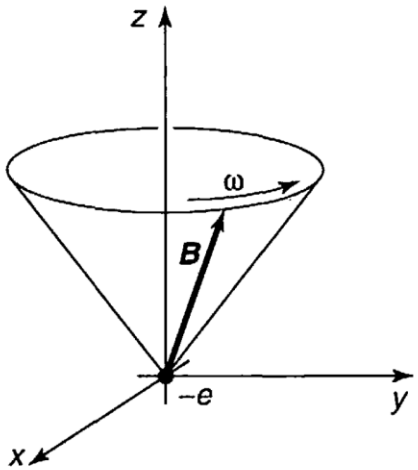
Assume electron is in state "n" at time t=0:

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

The solution tells us that all coefficients with n≠m remain 0 while the coefficient "n" acquires a phase factor. Thus, overall:

$$\Psi(t) = \sum_n c_n(t) \psi_n(t) e^{i\theta_n(t)} \longrightarrow \boxed{\Psi_n(t) = e^{i\theta_n(t)} e^{i\gamma_n(t)} \psi_n(t)}$$

Example 10.1. 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 :



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

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

$$H(t) = \frac{e}{m}\mathbf{B}\cdot\mathbf{S} = \frac{e\hbar B_0}{2m}[\sin\alpha\cos(\omega t)\sigma_x + \sin\alpha\sin(\omega t)\sigma_y + \cos\alpha\sigma_z]$$

$$= \frac{\hbar\omega_1}{2}\begin{pmatrix} \cos\alpha & e^{-i\omega t}\sin\alpha \\ e^{i\omega t}\sin\alpha & -\cos\alpha \end{pmatrix} \quad \text{with} \quad \omega_1 \equiv \frac{eB_0}{m}$$

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

$$\chi_+(t) = \begin{pmatrix} \cos(\alpha/2) \\ e^{i\omega t}\sin(\alpha/2) \end{pmatrix} \qquad \chi_-(t) = \begin{pmatrix} e^{-i\omega t}\sin(\alpha/2) \\ -\cos(\alpha/2) \end{pmatrix}$$

$$E_\pm = \pm\frac{\hbar\omega_1}{2}$$

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

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

Suppose the electron starts "up" along the direction of the field **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". In notes attached to solution of HW23, you will find 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 along the **B** direction:
(you will be asked to check this formula and next in HW23)

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

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

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

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:

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

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

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

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

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

$$\text{If} \quad \frac{\omega}{\omega_1} \to 0 \quad \text{then} \quad \lambda \equiv \sqrt{\omega^2 + \omega_1^2 - 2\omega\omega_1\cos\alpha} \longrightarrow \omega_1$$

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

For completeness, see Example 10.2 to separate dynamic vs geometric phases.