Physics 472 Lecture 22

The Adiabatic Approximation

An important situation in quantum mechanics is that of a Hamiltonian that changes "slowly" in time.

We have encountered this in the context of molecular dynamics, where we argued that the nuclear motion in a diatomic molecule was so much slower than the electronic motion, that it was a good approximation to "freeze" the nuclear motion when solving the electronic motion, then use the solution of the electronic problem as the input to solve the slower motion of the nuclei.

This adiabatic approximation is known, in the context of molecular dynamics, as the Born-Oppenheimer approximation.

The applications of the adiabatic approximation are sufficiently broad that we will study it as a general problem on its own.

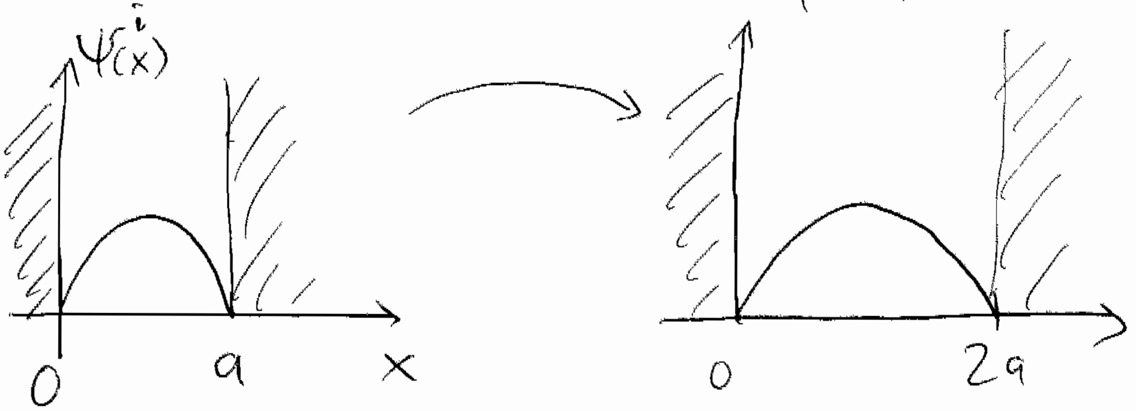
1) The Adiabatic theorem

Consider a Hamiltonian $H(t)$ that varies slowly with time s.t. $H(0) = H_i$ and $H(T) = H_f$.

(For simplicity, assume that the spectrum is discrete.)

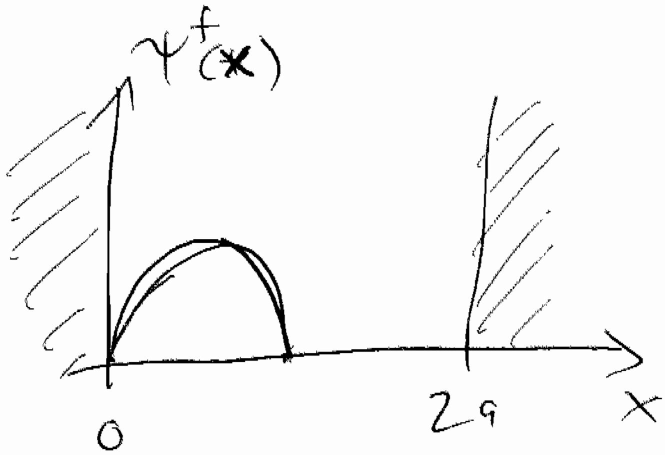
Then if the system is in the nth eigenstate of H_i at $t=0$, it will evolve (according to Schrödinger's equation) into the nth eigenstate of H_f at $t=T$.

<u>Example</u> Consider a particle in the ground state of a one-dimens. box:



If the right wall of the box is <u>slowly</u> moved outward from $x=a$ at $t=0$ to $x=2a$ at a later time $t=T$, then the wavefunction will be the ground state of the larger box. Energy is not conserved; the particle does work on the wall as it moves outward.

If, instead, the wall is suddenly moved to $x=2a$, the wavefunction would be:

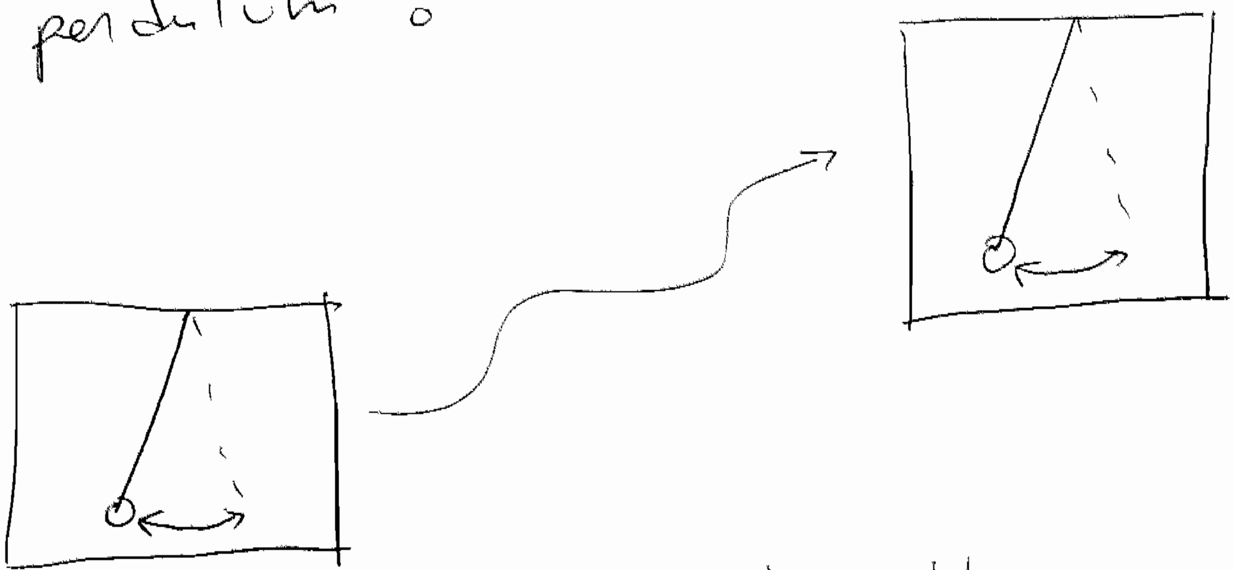


$$\psi^f(x, t=0^+) = \psi^i(x, t= \text{[illegible]}$$

<u>Sudden approx.</u>

$\Rightarrow$ Continuity

The proof of the adiabatic theorem is subtle. In fact, it is essentially a classical effect. A typical classical example is a slowly perturbed pendulum:



If the box containing the pendulum is moved about rapidly, the pendulum will fluctuate chaotically. However, if the box is moved slowly, the amplitude of the oscillation will be unaffected. In classical mechanics, the action

$S = \oint p\,dq$ is an adiabatic invariant (see any advanced text on classical mechanics).

In QM, the action is quantized $S = nh + \text{const.}$, so the classical invariance of the action implies that the quantum # is unchanged by an adiabatic process.

A slightly simpler classical example is a harmonic oscillator with a slowly-varying spring constant.

$$m \ddot{x} = - K(t)\, x$$

or $\ddot{x} = - \omega^2(t)\, x$, $\omega(t) = \sqrt{\frac{k(t)}{m}}$

$$E(t) = \frac{m \dot{x}^2}{2} + \frac{m \omega(t)^2}{2} x^2$$

$$\frac{dE}{dt} = m \dot{x} \ddot{x} + m \omega^2(t)\, x \dot{x} + m \omega \dot{\omega} x^2$$

$$= m \dot{x} \left(\cancelto{0}{\ddot{x} + \omega^2(t)\, x} \right) + m \omega \dot{\omega} x^2$$

An approximate solution is

$$x(t) = A(t) \cos\left(\omega(t)\, t + \delta(t)\right),$$

where $A(t)$, $\omega(t)$, and $\delta(t)$ vary slowly.

$$\bar{E} \simeq \frac{m \omega^2 A^2 \sin^2(\omega t + \delta)}{2} + \frac{m \omega^2 A^2 \cos^2(\omega t + \delta)}{2}$$

$$= \frac{m \omega^2 A^2}{2}$$ (average over one period)

$$\overline{\frac{dE}{dt}} = m\omega\dot{\omega}\,\overline{x^2} = m\omega\dot{\omega}\frac{A^2}{2}$$

$$\frac{\overline{\dot{E}}}{\overline{E}} = \frac{\dot{\omega}}{\omega}$$

Now $\quad S = \oint p\,dx = \oint m\dot{x}\,dx$

$$= m\int_0^{2\pi/\omega} \dot{x}^2\,dt \simeq \frac{m\omega^2 A^2}{2}\frac{2\pi}{\omega}$$

$$= \frac{2\pi\,\overline{E}}{\omega}.$$

So $\quad \dfrac{\dot{S}}{2\pi} = \dfrac{\overline{\dot{E}}}{\omega} - \dfrac{\overline{E}\,\dot{\omega}}{\omega^2} = \dfrac{\overline{E}}{\omega}\left(\dfrac{\overline{\dot{E}}}{\overline{E}} - \dfrac{\dot{\omega}}{\omega}\right)_0$

$$\boxed{\frac{dS}{dt} \simeq 0} \Rightarrow S \text{ is an adiabatic invariant.}$$

Combining this classical result with the Q.M. formula

$$E = \hbar\omega\left(n+\tfrac{1}{2}\right),$$

we get

$$2\pi\frac{E}{\omega} = h\left(n+\tfrac{1}{2}\right) \simeq \text{const.},$$

i.e., the quantum # n is conserved if ω varies slowly, i.e., if $\frac{\dot{\omega}}{\omega^2} \ll 1$.

2) General Proof of the Adiabatic Theorem

$$i\hbar\frac{\partial\Psi}{\partial t} = H(t)\,\Psi(t)$$

The eigenfunctions and eigenvalues of H are now time dependent:

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

The states $\psi_n(t)$ are not solutions of the time-dep. Schrödinger equation, but they do form a complete orthonormal basis in which to expand such a solution. Let us write

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

where

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

generalizes the usual time dependence to the case $E_n(t) \neq$ const.

Inserting $\Psi(t)$ into the Schrödinger equation yields

$$i\hbar \sum_n \left[\dot{c}_n \psi_n + c_n \dot{\psi}_n + \cancel{i c_n \psi_n \dot{\theta}_n} \right] e^{i\theta_n}$$

$$= \sum_n \cancel{c_n (H \psi_n)} e^{i\theta_n}$$

However $\dot{\theta}_n = -\dfrac{E_n(t)}{\hbar}$ so ,

which leaves

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

Taking the inner product with $\psi_m(t)$

gives

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

or

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

But differentiating the eigenvalue equation gives

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

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

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

or $\langle\psi_m|\dot{H}|\psi_n\rangle = (E_n - E_m)\langle\psi_m|\dot{\psi}_n\rangle + \dot{E}_n\,\delta_{nm}$

$$\Rightarrow \dot{c}_m(t) = -c_m\langle\psi_m|\dot{\psi}_m\rangle - \sum_{n\neq m} c_n \frac{\langle\psi_m|\dot{H}|\psi_n\rangle}{E_n - E_m}\, e^{i(\theta_n - \theta_m)}$$

This result is exact. The <u>adiabatic approx.</u> consists in dropping the term involving $\dot{H}$:

$$\dot{c}_m(t) \simeq -c_m\langle\psi_m|\dot{\psi}_m\rangle$$

The solution is

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

where

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

(Notice that γ_m is real since

$$\frac{d}{dt}\langle \psi_m | \psi_m \rangle = \langle \psi_m | \dot{\psi}_m \rangle + \langle \dot{\psi}_m | \psi_m \rangle$$

$$= 2\,\mathrm{Re}\,\langle \psi_m | \dot{\psi}_m \rangle = 0 \Big).$$

In particular, if the system starts out in a particular eigenstate ψ_n, i.e., $c_m(0) = \delta_{nm}$, then

$$\Psi(t) = e^{i\theta_n(t)}\, e^{i\gamma_n(t)}\, \psi_n(t).$$

The system remains in the nth eigenstate, picking up only the multiplicative phase factors.