The adiabatic theorem

The adiabatic approximation plays an important role and has many applications in physics. In quantum mechanics the essential content of the adiabatic approximation can be cast into a form of a theorem:

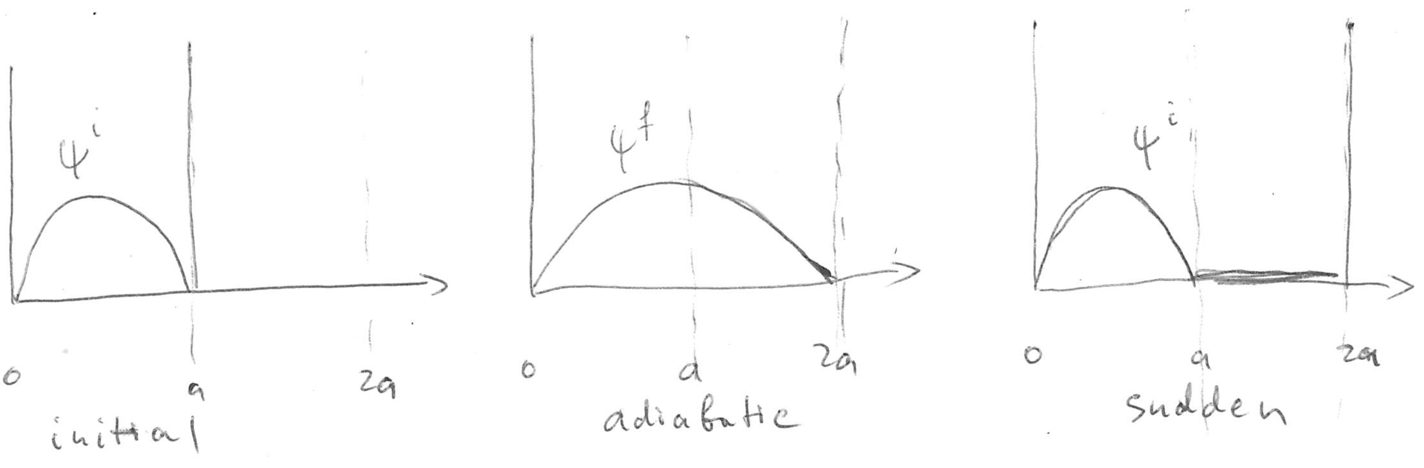
Suppose the Hamiltonian changes gradually from some initial form H^i to some final form H^f. Then if the system was initially in the n-th eigenstate of H^i, it will be carried into the n-th eigenstate of H^f (assuming that the spectrum is discrete and nondegenerate throughout the transition from H^i to H^f)

Consider, for example a particle in the ground state of the infinite square well:

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

If we gradually move the right wall out to $2a$ the particle will end up in the ground state of the expanded well

$$\psi^f(x) = \sqrt{\frac{1}{a}} \sin \frac{\pi x}{2a}$$ (apart from, perhaps, a phase factor)



Energy is not conserved — whoever is moving the wall is extracting energy from the system. By contrast, if the wall is expanded suddenly, the resulting state is still φ^i, which is a complicated linear combination of eigenstates of the new Hamiltonian. In this case the energy is conserved (its expectation value). This is similar to the free expansion of a gas into vacuum when the barrier is suddenly removed — no work is done.

Let us prove the adiabatic theorem

If H is independent of time, then a particle which starts out in the n-th state φ_n

$$H\varphi_n = E_n\varphi_n$$

remains in the n-th state indefinitely, simply picking up a phase factor $\Phi_n = \varphi_n e^{-\frac{iE_n t}{\hbar}}$

Now if H changes with time then

$$H(t)\,\varphi_n(t) = E_n(t)\,\varphi_n(t)$$ ← eigenfunctions and eigenenergies are time-dependent

However, at any time

$$\langle \varphi_n(t) | \varphi_m(t) \rangle = \delta_{nm}$$

and $\{\varphi_n(t)\}$ form a complete set so that the general solution to the time-dependent Schrödinger equation can be expressed as a linear combination

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

where $\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\,dt'$ generalizes the standard phase factor

(This phase factor could be included into $c_n(t)$ but it is convenient to factor it out)

Substituting $\Psi(t)$ into the TDSE we obtain

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

$$i\hbar \sum_n \left[\dot{c}_n \varphi_n + c_n \dot{\varphi}_n + i c_n \varphi_n \dot{\theta}_n\right] e^{i\theta_n} = \sum_n c_n (H\varphi_n) e^{i\theta_n}$$

The last two term cancel because we recall that

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

Then

$$\sum_n \dot{c}_n |\varphi_n\rangle e^{i\theta_n} = -\sum_n c_n |\dot{\varphi}_n\rangle e^{i\theta_n}$$

multiplying by $\langle\varphi_m|$ we get

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

or

$$\dot{c}_m(t) = -\sum_n c_n \langle\varphi_m|\dot{\varphi}_n\rangle e^{i(\theta_n-\theta_m)} \qquad (*)$$

Now differendiating $H(t)\varphi_n(t) = E_n(t)\varphi_n(t)$ with respect to time yields:

$$\dot{H}\varphi_n + H\dot{\varphi}_n = \dot{E}_n\varphi_n + E_n\dot{\varphi}_n$$

Taking a product with $\langle\varphi_m|$ we get

$$\langle\varphi_m|\dot{H}|\varphi_n\rangle + \langle\varphi_m|H|\dot{\varphi}_n\rangle = \dot{E}_n\delta_{mn} + E_n\langle\varphi_m|\dot{\varphi}_n\rangle$$

Since $\langle\varphi_m|H|\dot{\varphi}_n\rangle = E_m\langle\varphi_m|\dot{\varphi}_n\rangle$ it follows that for $n \neq m$

$$\langle\varphi_m|\dot{H}|\varphi_n\rangle = (E_n - E_m)\langle\varphi_m|\dot{\varphi}_n\rangle$$

Putting this into equation (*) and assuming for simplicity that the energies are nondegenerate we get

$$\dot{c}_m(t) = -c_m\langle \varphi_m|\dot{\varphi}_m\rangle - \sum_{n\neq m} c_n \frac{\langle \varphi_m|\dot{H}|\varphi_n\rangle}{E_n - E_m} e^{-\frac{i}{\hbar}\int_0^t (E_n(t') - E_m(t'))\,dt'}$$

Up to this point we have made no approximations. If E_m is well separated from E_n, then all terms in the sum are oscillating rapidly in comparison with $\langle \varphi_m|\dot{\varphi}_m\rangle$ (which changes infinitely slowly). Thus, we can neglect the sum for time scales $T \gg \frac{\hbar}{E_n - E_m}$ and

$$\dot{c}_m(t) = -c_m\langle \varphi_m|\dot{\varphi}_m\rangle$$

with the solution

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

In particular if $c_n(0) = 1$ and $c_m(0) = 0$ $(m \neq n)$ then

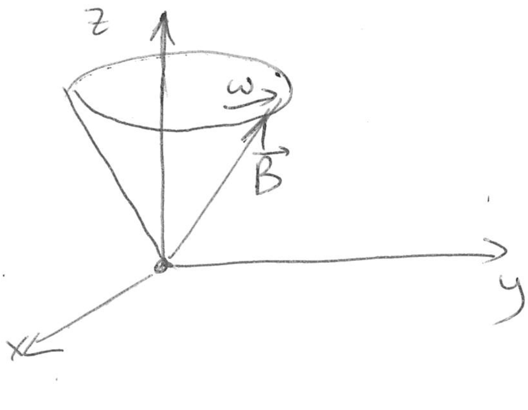
$$\Psi_n(t) = e^{i\theta_n(t)}\, e^{i\gamma_n(t)}\, \varphi_n(t)$$

The particle which starts out in the n-th state remains in the n-th state (of the evolving Hamiltonian) picking up only a couple of phase factors.

This ends the proof of the adiabatic theorem.

Now let us consider an example of an adiabatic transition — an electron placed in a magnetic field whose magnitude is constant while the direction sweeps out a cone of opening angle α at a constant angular velocity ω

$$\vec{B}(t) = B_0\left[\sin\alpha\cos\omega t\,\hat{i} + \sin\alpha\sin\omega t\,\hat{j} + (\cos\alpha)\hat{k}\right.$$



The Hamiltonian is

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

$$= \frac{\hbar\omega_0}{2}\begin{pmatrix}\cos\alpha & e^{-i\omega t}\sin\alpha \\ e^{i\omega t}\sin\alpha & -\cos\alpha\end{pmatrix} \qquad \text{where} \qquad \omega_0 = \frac{eB_0}{m}$$

The normalized eigenspinors are

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

They represent spin up and spin down states, respectively, along the instantaneous direction of $\vec{B}(t)$. The corresponding eigenvalues are $E_\pm = \pm\frac{\hbar\omega_0}{2}$

Suppose the electron starts out with spin up, along $\vec{B}(0)$:

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

The exact solution to the TDSE is

$$\chi(t) = \begin{pmatrix}\left[\cos\left(\frac{\lambda t}{2}\right) - i\,\frac{\omega_0-\omega}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\cos\frac{\alpha}{2}\,e^{-\frac{i\omega t}{2}} \\ \left[\cos\left(\frac{\lambda t}{2}\right) - i\,\frac{\omega_0-\omega}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]\sin\frac{\alpha}{2}\,e^{+\frac{i\omega t}{2}}\end{pmatrix}$$

where $\lambda = \sqrt{\omega^2 + \omega_0^2 - 2\omega\omega_0\cos\alpha}$

It can be represented as a linear combination of χ_+ and χ_-:

$$\chi(t) = \left[\cos\frac{\lambda t}{2} - i\,\frac{\omega_0 - \omega\cos\alpha}{\lambda}\sin\left(\frac{\lambda t}{2}\right)\right]e^{-\frac{i\omega t}{2}}\chi_+(t)$$

$$+ i\left[\frac{\omega}{\lambda}\sin\alpha\sin\frac{\lambda t}{2}\right]e^{+\frac{i\omega t}{2}}\chi_-(t)$$

Exact probability of transition to spin down state (along current $\vec{B}$) is

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

The adiabatic theorem says this transition should vanish in the limit $T_e >> T_i$ (where T_e and T_i are characteristic time for changes in the hamiltonian and the wave function, respectively).

$$T_e \sim \frac{1}{\omega}$$

$$T_i \sim \frac{\hbar}{E_+ - E_-} = \frac{1}{\omega_0}$$

Thus in the adiabatic approximation we require that $\omega << \omega_0$ and $\lambda \simeq \omega_0$

Then

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

The magnetic field leads the electron around by its nose. The spin is always in the direction of $\vec{B}$.

In contrast, if $\omega >> \omega_0$ and $\lambda \simeq \omega$ the system bounces forth and back between spin up and spin down states