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 inte form of a theorem:

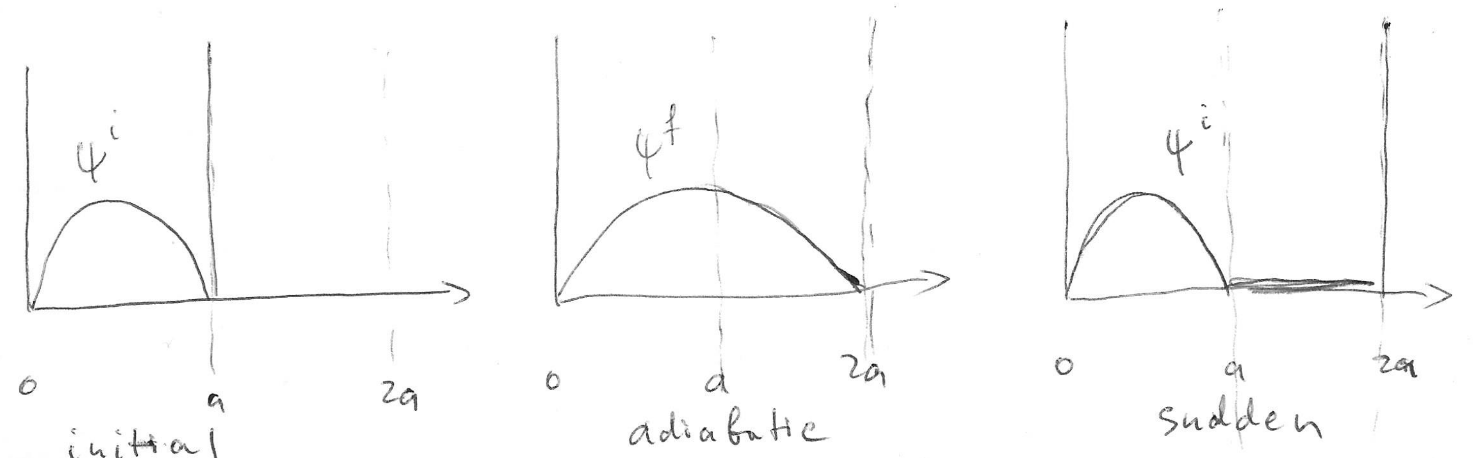
Suppose the Hamiltonian changes gradually from some initial form H^i to some final form H^f. Then if the system was initially in the n-th eigenstate of H^i, it will be carried into the n-th eigenstate of H^f (assuming that the spectrum is discrete and nondegenerate throughout the transition from H^i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

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

with the solution

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

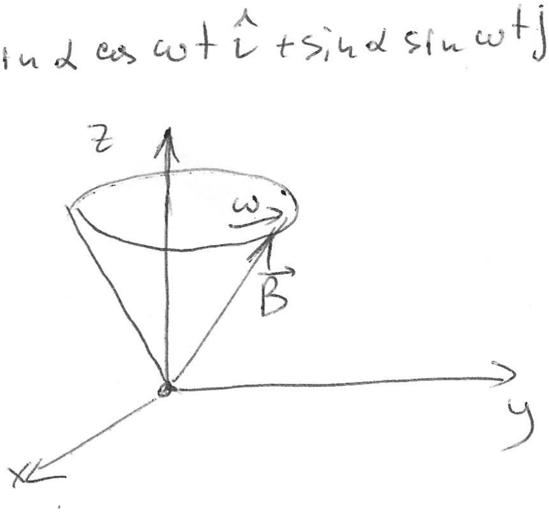
In particular if $c_n(0) = 1$ and $c_m(0) = 0$ $(m\neq n)$ then

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

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