THE ADIABATIC APPROXIMATION IN QUANTUM MECHANICS

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 10.1.

The adiabatic approximation in quantum mechanics is a method by which approximate solutions to the time dependent Schrödinger equation can be found. The method works in cases where the hamiltonian changes slowly by comparison with the natural, internal frequency of the wave function. For example, the general solution to the time-independent Schrödinger equation can be written as

$$\Psi(x,t)=\sum_{n}c_{n}\psi_{n}(x)\,e^{-iE_{n}t/\hbar} \tag{1}$$

where the $\psi_n(x)$ are the eigenfunctions of the hamiltonian with eigenvalues (energies) E_n. The internal frequency of eigenfunction n is $E_n/\hbar$, so if the variations in the hamiltonian have frequency components much lower than this, we can use the adiabatic approximation.

The adiabatic theorem states that in a system with non-degenerate energy levels, if we start with the system in level n of the original hamiltonian and then undergo an adiabatic process that takes us to some final hamiltonian, then the system will be in level n of the final hamiltonian, although the wave function may pick up a phase factor along the way.

A common example of an adiabatic process is an infinite square well that starts with width a that increases slowly over time with constant speed v so that the width is given by

$$w(t)=a+vt \tag{2}$$

for $t\ge 0$. If we let the wall expand to twice its original width, then we can take as the 'external' time T_e the time it takes to complete its expansion:

$$T_e=\frac{a}{v} \tag{3}$$

The 'internal' time T_i can be the period of the phase factor $e^{-iE_n t/\hbar}$ in the starting state, so we would have

$$\frac{E_n T_i}{\hbar} = 2\pi \tag{4}$$

$$T_i = \frac{2\pi\hbar}{E_n} \tag{5}$$

However, it turns out that the time dependent Schrödinger equation can be solved exactly in this case, with the nth eigenfunction given by

$$\Phi_n(x,t) = \sqrt{\frac{2}{w}} \sin\left(\frac{n\pi}{w}x\right) e^{i\left(mvx^2 - 2E_n^i at\right)/2\hbar w} \tag{6}$$

where E_n^i is the energy of level n in the starting well, with width a:

$$E_n^i = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{7}$$

We can verify by direct differentiation that 6 satisfies the time dependent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Phi_n}{\partial x^2} = i\hbar\frac{\partial\Phi_n}{\partial t} \tag{8}$$

The calculation gets very messy (remember w depends on t) so it's best to use Maple to do it, and we get

$$i\hbar\frac{\partial\Phi_n}{\partial t} = e^{i\left(mvx^2 - 2E_n^i at\right)/2\hbar w}\frac{\sqrt{2}}{w^{5/2}}\left[\frac{1}{2}\sin\left(\frac{n\pi}{w}x\right)\left(\frac{(n\pi\hbar)^2}{m} + m(vx)^2 - i\hbar vw\right) - i\cos\left(\frac{n\pi}{w}x\right)\pi n\hbar vx\right] \tag{9}$$

Fortunately, we get the same expression for $-\frac{\hbar^2}{2m}\frac{\partial^2\Phi_n}{\partial x^2}$ so the Schrödinger equation is satisfied.

6 is the wave function for a single energy level, so we can get a general solution that is a superposition of energy levels in the usual way:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Phi_n(x,t) \tag{10}$$

In this case, all the time dependence is included in the Φ_n, so the coefficients c_n are true constants, independent of both space and time. The Φ_n are orthonormal at each instant of time, since

$$\int_0^w \Phi_j^* \Phi_n dx = \frac{2}{w} e^{2iat\left(E_j^i - E_n^i\right)/2\hbar w} \int_0^w \sin\left(\frac{j\pi}{w}x\right) \sin\left(\frac{n\pi}{w}x\right) dx \tag{11}$$

$$= e^{2iat\left(E_j^i - E_n^i\right)/2\hbar w} \delta_{jn} \tag{12}$$

$$= \delta_{jn} \tag{13}$$

We can therefore use orthonormality to get an expression for c_n by multiplying both sides by Φ_j^* and integrating. Since the c_n are independent of time, we can do this at $t = 0$ when $w = a$.

$$c_j = \int_0^a \Phi_j^* (x,0) \Psi(x,0) dx \tag{14}$$

If the particle starts out in the ground state, then

$$\Psi(x,0) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right) \tag{15}$$

$$c_n = \frac{2}{a} \int_0^a e^{-imvx^2/2\hbar a} \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{\pi}{a}x\right) dx \tag{16}$$

Substituting $z = \pi x/a$ we get

$$c_n = \frac{2}{\pi} \int_0^\pi e^{-i\alpha z^2} \sin(nz) \sin(z) dz \tag{17}$$

$$\alpha \equiv \frac{mva}{2\pi^2 \hbar} \tag{18}$$

So far, all this is exact. To use the adiabatic approximation, we need estimates of T_e and T_i. We can get T_e from 3. For T_i we can look at 6 at $x = 0$ and find the value of t that makes the argument of the exponential advance by 2π. Actually, because of the signs, the phase actually goes backwards as t gets larger, but the principle is the same; we just need to find the value of t at which the argument changes by 2π.

$$\frac{2E_1^i a T_i}{2\hbar (a + vT_i)} = 2\pi \tag{19}$$

$$T_i = \frac{2\pi\hbar a}{E_1^i a - 2\pi\hbar v} \tag{20}$$

Dividing top and bottom by v and using 3 we get

$$T_i = \frac{2\pi\hbar T_e}{E_1^i T_e - 2\pi\hbar} \tag{21}$$

To satisfy the adiabatic condition, we need $T_e \gg T_i$ so, using 7

$$\begin{aligned} \frac{2\pi\hbar}{E_1^i T_e - 2\pi\hbar} &\ll 1 && (22) \\ E_1^i T_e &\gg 4\pi\hbar && (23) \\ \frac{8mav}{\pi\hbar} &\ll 1 && (24) \end{aligned}$$

Apart from the numerical factors which don't differ too drastically, we see from 18 that this effectively requires $\alpha \ll 1$. Using this approximation, we can evaluate the integral in 17 to get

$$\begin{aligned} c_n &\approx \frac{2}{\pi}\int_0^\pi \sin(nz)\sin(z)\,dz && (25) \\ &= \delta_{1n} && (26) \end{aligned}$$

Thus the system remains in the ground state $n = 1$ as the wall expands, which is what the adiabatic theorem predicts. The wave function is therefore

$$\Phi_1(x,t) \approx \sqrt{\frac{2}{w}}\sin\left(\frac{\pi}{w}x\right)e^{i\left(mvx^2 - 2E_1^i at\right)/2\hbar w} \tag{27}$$

The phase factor in this wave function is the exponential factor that doesn't depend on x, that is

$$\theta(t) = -\frac{2E_1^i at}{2\hbar w} = -\frac{\pi^2\hbar t}{2ma(a+vt)} \tag{28}$$

The instantaneous eigenvalue in the ground state is the original eigenvalue with the well width a replaced by the dynamic width w:

$$E_1(t) = \frac{\pi^2\hbar^2}{2mw^2} \tag{29}$$

If we integrate this over the time the wall has moved so far we get

$$\int_0^t E_1(t')\,dt' = \frac{\pi^2\hbar^2}{2m}\int_0^t \frac{dt'}{(a+vt')^2} \tag{30}$$

$$= \frac{\pi^2\hbar^2 t}{2ma(a+vt)} \tag{31}$$

$$= -\hbar\theta(t) \tag{32}$$

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