ADIABATIC APPROXIMATION: HIGHER ORDER CORRECTIONS

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 10.10.

In deriving the adiabatic theorem, Griffiths (in his section 10.1) shows that the solution to the time-dependent Schrödinger equation can be written as

$$\Psi(x,t) = \sum_n c_n(t)\,\psi_n(x,t)\,e^{i\theta_n(t)} \tag{0.1}$$

where the ψ_n form an orthonormal set of functions that are eigenfunctions of the Hamiltonian at a particular instant of time, and θ_n is the dynamic phase. The coefficients c_n are the usual weighting factors, and they depend only on time.

Later in the derivation, he arrives at a differential equation for the c_m:

$$\dot{c}_m(t) = -\sum_j c_j \left\langle \psi_m \middle| \dot{\psi}_j \right\rangle e^{i\left(\theta_j - \theta_m\right)} \tag{0.2}$$

In the adiabatic approximation, this equation has the approximate solution

$$c_m(t) = c_m(0)\,e^{i\gamma_m(t)} \tag{0.3}$$

$$\gamma_m(t) \equiv i\int_0^t \left\langle \psi_m\left(t'\right) \middle| \frac{\partial}{\partial t'}\psi_m\left(t'\right) \right\rangle dt' \tag{0.4}$$

where γ_m is the geometric phase. In particular, if the system starts in a definite eigenstate ψ_n then $c_m(0) = \delta_{nm}$ so

$$c_m(t) = \delta_{nm} e^{i\gamma_n(t)} \tag{0.5}$$

with the result that the overall solution becomes

$$\Psi_n(x,t) = \psi_n(x,t)\,e^{i\theta_n(t)}e^{i\gamma_n(t)} \tag{0.6}$$

that is, the system stays in the n^{th} state over time, although its phase can change.

We can extend the adiabatic approximation recursively by using the first approximation 0.5 to generate the next approximation. We can do this by inserting 0.5 into 0.2 and then solving the resulting differential equation. The sum in 0.2 is reduced to a single term where $j = n$, the eigenstate in which the system starts at $t = 0$.

$$\dot{c}_m(t) = -e^{i\gamma_n(t)} \langle \psi_m | \dot{\psi}_n \rangle e^{i(\theta_n - \theta_m)} \tag{0.7}$$

$$c_m(t) = c_m(0) - \int_0^t e^{i\gamma_n(t)} \langle \psi_m | \dot{\psi}_n \rangle e^{i(\theta_n - \theta_m)} dt' \tag{0.8}$$

This correction to the basic adiabatic approximation now has the ability to predict transitions from the initial state ψ_n to other states ψ_m where $m \neq n$. We can apply this to the forced oscillator, where we found that in the adiabatic approximation

$$\psi_n(x,t) = \psi_n(x-f) \tag{0.9}$$

$$\theta_n(t) = \frac{m\omega^2}{2\hbar} \int_0^t f^2(t')\, dt' - \left(n + \frac{1}{2}\right) \omega t \tag{0.10}$$

$$\gamma_n(t) = \frac{m\dot{f}}{\hbar} \left(x - \frac{f}{2}\right) \approx 0 \tag{0.11}$$

Here, $m\omega^2 f(t)$ is the forcing term, and the adiabatic approximation is obtained by assuming that f changes very slowly, or to be precise:

$$\left|\dot{f}(t)\right| \ll \omega |f(t)| \tag{0.12}$$

To work out the correction, we need to find $\langle \psi_m | \dot{\psi}_n \rangle$ in 0.8. We can do this using the raising and lowering operators for the harmonic oscillator. In particular, the momentum operator can be written in terms of them as

$$p = i\sqrt{\frac{\hbar m\omega}{2}} (a_+ - a_-) \tag{0.13}$$

Also, recall that the effects of $a_\pm$ are

$$a_+ \psi_n = \sqrt{n+1}\, \psi_n \tag{0.14}$$

$$a_- \psi_n = \sqrt{n}\, \psi_{n-1} \tag{0.15}$$

How does this help us? We need to find the derivative $\partial \psi_n(x-f)/\partial t'$, so we get, defining $z \equiv x - f$:

$$\frac{\partial \psi_n(x-f)}{\partial t'} = \frac{\partial \psi_n(z)}{\partial z}\frac{\partial z}{\partial t'} \tag{0.16}$$

$$= -\frac{\partial \psi_n(z)}{\partial z}\dot{f} \tag{0.17}$$

$$= -\frac{\partial \psi_n}{\partial x}\dot{f} \tag{0.18}$$

where the last line follows because $z = x - f$ and f doesn't depend on x.
Now the momentum operator is

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{0.19}$$

so our derivative is

$$\frac{\partial \psi_n(x-f)}{\partial t'} = -\frac{i}{\hbar}\dot{f}p\psi_n \tag{0.20}$$

$$= \dot{f}\sqrt{\frac{m\omega}{2\hbar}}(a_+ - a_-)\psi_n \tag{0.21}$$

$$= \dot{f}\sqrt{\frac{m\omega}{2\hbar}}\left(\sqrt{n+1}\psi_{n+1} - \sqrt{n}\psi_{n-1}\right) \tag{0.22}$$

Using the orthonormality of the ψ_m we have

$$\langle \psi_{n+1} | \dot{\psi}_n \rangle = \dot{f}\sqrt{\frac{m\omega}{2\hbar}}\sqrt{n+1} \tag{0.23}$$

$$\langle \psi_{n-1} | \dot{\psi}_n \rangle = -\dot{f}\sqrt{\frac{m\omega}{2\hbar}}\sqrt{n} \tag{0.24}$$

with all other matrix elements equal to zero.
Returning to 0.8 we can work out the phase terms from 0.10 and 0.11.

$$\gamma_n \approx 0 \tag{0.25}$$

$$\theta_n - \theta_{n+1} = \omega t \tag{0.26}$$

$$\theta_n - \theta_{n-1} = -\omega t \tag{0.27}$$

Therefore, since $c_{n+1}(0) = c_{n-1}(0) = 0$,

$$c_{n+1}(t) = -\sqrt{\frac{m\omega}{2\hbar}}\sqrt{n+1}\int_0^t \dot{f}e^{i\omega t'}dt' \tag{0.28}$$

$$c_{n-1}(t) = \sqrt{\frac{m\omega}{2\hbar}}\sqrt{n}\int_0^t \dot{f}e^{-i\omega t'}dt' \tag{0.29}$$

[These answers aren't the same as those given in Griffiths's question (although the square moduli are the same) but I can't see anything wrong with my derivation. Comments welcome.]

Note that

$$\langle \psi_n | \dot{\psi}_n \rangle = 0 \tag{0.30}$$

so 0.8 predicts that $c_n(t) = c_n(0) = 1$, thus the sum of the square moduli of the c_ms is greater than 1. However, these values for the c_ms are correct only to first order in $\dot{f}$. To get the second order corrections, we'd need to insert 0.28 and 0.29 back into 0.2 and integrate again to get new values for the c_ms, which would give $c_n(t) < 1$ for $t > 0$. The process can be continued as long as we like, giving an adiabatic series.