

## 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

$$\Psi(x, t) = \sum_n c_n(t) \psi_n(x, t) e^{i\theta_n(t)} \quad (1)$$

where the  $\psi_n$  form an orthonormal set of functions that are eigenfunctions of the Hamiltonian at a particular instant of time, and  $\theta_n$  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  $c_m$ :

$$\dot{c}_m(t) = - \sum_j c_j \langle \psi_m | \dot{\psi}_j \rangle e^{i(\theta_j - \theta_m)} \quad (2)$$

In the adiabatic approximation, this equation has the approximate solution

$$c_m(t) = c_m(0) e^{i\gamma_m(t)} \quad (3)$$

$$\gamma_m(t) \equiv i \int_0^t \left\langle \psi_m(t') \left| \frac{\partial}{\partial t'} \psi_m(t') \right. \right\rangle dt' \quad (4)$$

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

$$c_m(t) = \delta_{nm} e^{i\gamma_m(t)} \quad (5)$$

with the result that the overall solution becomes

$$\Psi_n(x, t) = \psi_n(x, t) e^{i\theta_n(t)} e^{i\gamma_n(t)} \quad (6)$$

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

We can extend the adiabatic approximation recursively by using the first approximation 5 to generate the next approximation. We can do this by

inserting 5 into 2 and then solving the resulting differential equation. The sum in 2 is reduced to a single term where  $j = n$ , the eigenstate in which the system starts at  $t = 0$ .

$$\dot{c}_m(t) = -e^{i\gamma_n(t)} \langle \psi_m | \dot{\psi}_n \rangle e^{i(\theta_n - \theta_m)} \quad (7)$$

$$c_m(t) = c_m(0) - \int_0^t e^{i\gamma_n(t')} \langle \psi_m | \dot{\psi}_n \rangle e^{i(\theta_n - \theta_m)} dt' \quad (8)$$

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

$$\psi_n(x, t) = \psi_n(x - f) \quad (9)$$

$$\theta_n(t) = \frac{m\omega^2}{2\hbar} \int_0^t f^2(t') dt' - \left(n + \frac{1}{2}\right) \omega t \quad (10)$$

$$\gamma_n(t) = \frac{m\dot{f}}{\hbar} \left(x - \frac{f}{2}\right) \approx 0 \quad (11)$$

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:

$$|\dot{f}(t)| \ll \omega |f(t)| \quad (12)$$

To work out the correction, we need to find  $\langle \psi_m | \dot{\psi}_n \rangle$  in 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

$$p = i\sqrt{\frac{\hbar m\omega}{2}} (a_+ - a_-) \quad (13)$$

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

$$a_+ \psi_n = \sqrt{n+1} \psi_{n+1} \quad (14)$$

$$a_- \psi_n = \sqrt{n} \psi_{n-1} \quad (15)$$

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

$$\frac{\partial \psi_n(x-f)}{\partial t'} = \frac{\partial \psi_n(z)}{\partial z} \frac{\partial z}{\partial t'} \quad (16)$$

$$= -\frac{\partial \psi_n(z)}{\partial z} \dot{f} \quad (17)$$

$$= -\frac{\partial \psi_n}{\partial x} \dot{f} \quad (18)$$

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

$$p = \frac{\hbar}{i} \frac{\partial}{\partial x} \quad (19)$$

so our derivative is

$$\frac{\partial \psi_n(x-f)}{\partial t'} = -\frac{i}{\hbar} \dot{f} p \psi_n \quad (20)$$

$$= \dot{f} \sqrt{\frac{m\omega}{2\hbar}} (a_+ - a_-) \psi_n \quad (21)$$

$$= \dot{f} \sqrt{\frac{m\omega}{2\hbar}} (\sqrt{n+1} \psi_{n+1} - \sqrt{n} \psi_{n-1}) \quad (22)$$

Using the orthonormality of the  $\psi_m$  we have

$$\langle \psi_{n+1} | \dot{\psi}_n \rangle = \dot{f} \sqrt{\frac{m\omega}{2\hbar}} \sqrt{n+1} \quad (23)$$

$$\langle \psi_{n-1} | \dot{\psi}_n \rangle = -\dot{f} \sqrt{\frac{m\omega}{2\hbar}} \sqrt{n} \quad (24)$$

with all other matrix elements equal to zero.

Returning to 8 we can work out the phase terms from 10 and 11.

$$\gamma_n \approx 0 \quad (25)$$

$$\theta_n - \theta_{n+1} = \omega t \quad (26)$$

$$\theta_n - \theta_{n-1} = -\omega t \quad (27)$$

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

$$c_{n+1}(t) = -\sqrt{\frac{m\omega}{2\hbar}} \sqrt{n+1} \int_0^t \dot{f} e^{i\omega t'} dt' \quad (28)$$

$$c_{n-1}(t) = \sqrt{\frac{m\omega}{2\hbar}} \sqrt{n} \int_0^t \dot{f} e^{-i\omega t'} dt' \quad (29)$$

[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

$$\langle \psi_n | \dot{\psi}_n \rangle = 0 \quad (30)$$

so 8 predicts that  $c_n(t) = c_n(0) = 1$ , thus the sum of the square moduli of the  $c_m$ s is greater than 1. However, these values for the  $c_m$ s are correct only to first order in  $\dot{f}$ . To get the second order corrections, we'd need to insert 28 and 29 back into 2 and integrate again to get new values for the  $c_m$ s, which would give  $c_n(t) < 1$  for  $t > 0$ . The process can be continued as long as we like, giving an adiabatic series.