Time-independent perturbation theory

Introduction

The exercises today will deal with perturbation theory. We will start with a very simple example, taken straight out of David Griffiths' Quantum Mechanics, Third Edition, specifically Chapter 7. Then, we will move on to Problem 7.1 in Griffiths, but using Composer, we can explore much more than what Griffiths asks us to calculate.'

The goal of these exercises is for you to gain an understanding of how perturbation theory works and what it means to be "perturbative." That is, when does perturbation theory fail?

The Composer flowfile that we will use in the second exercise can be changed to model any potential and any perturbation, so feel free to test it with other problems. For example, what changes if you use a finite square well? How about if you were to change the sign of the perturbation so that instead of a delta function bump, you had a delta function dip? You can use this to study for the exam–change the problem a little bit, then try to calculate the solution. Use Composer to check your answers!

Lifting the infinite square well

Open the flowfile *ComposerPT1.flow*.

There are three potentials here. One is the infinite square well that you know and love, and the other two are `box()` potentials that represent our perturbations. One of the boxes lifts the whole potential as shown in Griffiths Figure 7.2, and the other only lifts half of the potential, as in Griffiths Figure 7.2.

Remember that in Composer, $\hbar = m = 1$.

1. We have cleverly chosen the width of the well to be $a = \pi$. Calculate the eigenenergies of the infinite square well. Check your answer in Composer.

The differences in the calculated energy and that shown in Composer are due to numerical errors. You can test this by changing the value of *n* in the "Spatial Dimension" box. Increasing *n* makes Composer's result closer to the real value, so we know the errors are numerical.

For the full-offset case shown in Fig. 7.1, Griffiths says that the first-order correction to the energy is simply equal to the offset V_0 (in Composer, this is written as `V0`). For the half-offset case shown in Fig. 7.2, the first-order correction gives $V_0/2$ Play with different values of V_0 and observe what happens to the energies.

2. How good is the first-order correction in the case of the full-offset to the well? Why?

3. How good is the first-order correction in the case of the half-offset well? Why is this different from the full offset well?

4. Play with different values of V_0. In what range of values is the perturbative result for the lowest-energy state valid to within 1%? 10%?

5. Answer the previous question again, but consider instead the first excited state (second-lowest energy state).

6. Why is the range of validity different for the two states? (Hint: Think about the energy of the state relative to the energy of the perturbation.)

Griffiths Problem 7.1 (and beyond!)

Open the flowfile *ComposerPT2.flow*.

Here, we have estimated a delta function potential as a very thin box. We won't ask you to calculate the answers, but it may be a good way to practice for the exam and compare (for example, you can explore the following question: how thin does the box have to be to best approximate a delta function).

Note that our system is a little bit different than Griffiths in that we center the well around zero, but he centers his around $a/2$. The answers you get should be the same, though!

First we will look at the corrections to the energies.

1. In Composer, do Problem 7.1(a). You can find the perturbed energies labelled as `dEn` in Composer, where $n = 0, .., 4$. In particular, explain why the values for $n = 1$ and 3 are almost zero. (These are the "even states" that Griffiths mentions.
2. How do the corrections to the energies that you found scale as you increase the values of α? (It may be helpful to use Excel or another plotting program to plot the corrections as a function of α.) Looking at Eq. (6.9) in Griffiths, does this scaling make sense?

Now we will look at the correction to the state. The comments in the flow file takes you step-by-step through the calculation that we have Composer do. Note that at the very end of the calculation, you have to write in the correct values of the linear combination by hand! This tells Composer how to do the sum in Griffiths Eq. (7.13) to get the right expression for the corrected state. (It's okay to enter the values up to three decimal places.)

3. Find the first-order correction to the ground state for delta function width $b = 0.1$ and $\alpha = 2$. In what ways is the state you found with perturbation theory similar or different to the exact result?
4. Change the values of α and do the above again (remember to change the values by hand!). For what values of α is the fidelity above 99%? 90%?
5. What parts of the state are the most difficult for the perturbative expansion to get right? (That is, is the difference between the two states higher in the centre of the plot or toward the edges?)

Now change the location of the box (denoted by the parameter `c` in Composer). Set $c = 1$.

6. Are the even energies still zero? Why or why not?
7. Is the approximation to the ground state better or worse?