ODE Assignment 18

Two-State and Three-State Quantum-Mechanical Systems and One Last Resonance Problem

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Introduction

Schrodinger's Equation is

$$i\,\hbar\,\frac{\partial\psi}{\partial t} = H\,\psi$$

We are going to ignore units of energy and time, so just ignore the reduced Planck's constant, $\hbar$. Then Schrodinger's equation is

$$i\,\frac{\partial\psi}{\partial t} = H\,\psi$$

Would it not be incredibly nice if there were solutions of this equation with all the time dependence of ψ simply being

$$\psi(t) = \psi(0)\,e^{-i\,\omega t}$$

In which case Schrodinger's equation is just

$$\omega\,\psi(0) = H\,\psi(0)$$

This looks awfully simple. However, I haven't told you that ψ is a vector with an infinite number of rows, and that H is a matrix with an infinite number of rows and an infinite number of columns.

I also haven't mentioned that H might be time-dependent if there are time-varying external forces acting on the system, such as an incoming radio wave impinging on an atom. The atom would be the system. The radio wave would be the source of external forces (its electric and magnetic fields act on the charged particles in the atom). We are not going to worry about time-dependence. That means we won't be able to do nuclear magnetic resonance. Oh well.

Problem 1 — 2-State Systems

Sometimes you can ignore all but a few states in the system. Ignoring all but one state is boring. The system is just stuck in that state. But ignoring all but two already gets interesting.

The most general, time-independent two-by-two Hamiltonian is,

$$H = \begin{pmatrix} E_0 - \Delta E/2 & \epsilon + i\delta \\ \epsilon - i\delta & E_0 + \Delta E/2 \end{pmatrix}$$

where all the variables are real. You say: “That doesn’t look completely general. Why can’t the diagonal elements have imaginary parts? And why must the off-diagonal elements be complex conjugates of each other?” Them is the rules of quantum mechanics. Actually, that isn’t very satisfying. It turns out that them is the rules because if they weren’t obeyed, then probability would not be conserved.

(i) Find the eigenvalues and eigenvectors when $\delta = 0$. In other words, solve the eigenvalue problem

$$\omega\, \psi(0) = \begin{pmatrix} E_0 - \Delta E/2 & \epsilon \\ \epsilon & E_0 + \Delta E/2 \end{pmatrix} \psi(0)$$

(ii) Write down the most general solution for $\psi(t) = \begin{pmatrix} \psi_1(t) \\ \psi_2(2) \end{pmatrix}$. The most general solution is a linear combination of the two solutions you found in Part (i). You can see that $e^{-i E_0 t}$ multiplies both terms in your general solution. It turns out that an overall phase (even a time-dependent overall phase) is uninteresting. Simplify by setting $E_0 = 0$.

(iii) Find the particular solution with initial condition $\psi(0) = \begin{pmatrix} \psi_1(0) \\ \psi_2(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. This means the particle is for certain in the “upper” state at $t = 0$.

(iii) The probability of finding the particle in the upper state at a later time is the magnitude squared of the upper component of the vector (you will have to dust off some memory of complex numbers if “magnitude squared” doesn’t immediately ring a bell). It must be a real number between 0 and 1 because anything other than that makes no sense for a probability. Find the probability and arrange your answer in such a way that this is clear.

Problem 2 — 3-State Systems

Consider a system with one ground state and two excited states:

$$H = \begin{pmatrix} E_0 & 0 & 0 \\ 0 & E_1 & 0 \\ 0 & 0 & E_1 \end{pmatrix}$$

Suppose some small perturbation connects the ground state to either excited state

$$H = \begin{pmatrix} E_0 & \epsilon & \epsilon \\ \epsilon & E_1 & 0 \\ \epsilon & 0 & E_1 \end{pmatrix}$$

but does not connect the two excited states to each other.

What are the eigenvalues and eigenvectors of this system? There should be three since the eigenvector problem is now a cubic.

I encourage you to make the approximation $\epsilon \ll E_1 - E_0$ as it is not only an important case, it makes the algebra easier.

A second thing that makes the algebra easier is to notice that the two excited states enter the problem very symmetrically. When you compute the eigenvectors, you can exploit this. Instead of considering general eigenvectors,

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}$$

Consider eigenvectors of the form (symmetric and anti-symmetric in the excited states):

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_4 \\ \psi_4 \end{pmatrix}$$

and

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_4 \\ -\psi_4 \end{pmatrix}$$

Problem 3 — Resonance

The last problem on the exam was a resonance problem: Logan p. 245 #5.

We aren't going to get to the most important resonance problem in quantum mechanics, which is the problem of nuclear magnetic resonance (NMR). This problem was solved I.I. Rabi. It is what gives us the entire industry of magnetic resonance imaging (MRI) among other things.

As a way of preparing you for the NMR problem when you someday reach it, let us do some more on the last problem on the exam, for which there was sadly not enough time. Let us assume you got as far (in finding a particular solution) as writing out what Logan Eq. (4.45) tells us:

$$\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \Phi\begin{pmatrix} k_1 \\ k_2 \end{pmatrix} + \Phi \int_0^t \Phi^{-1}(s)\, \boldsymbol{f}(s)\, ds, \text{ where } \Phi(t) = \begin{pmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{pmatrix}, \quad \Phi^{-1}(s) = \begin{pmatrix} \cos s & -\sin s \\ \sin s & \cos s \end{pmatrix}, \text{ and } \boldsymbol{f}(s) = \begin{pmatrix} 0 \\ \cos \omega s \end{pmatrix}.$$

Of course, if your Φ was different than mine, then your Φ^{-1} will be different than mine too, because Φ is "a" fundamental matrix, not "the" fundamental matrix. Let's use my Φ and Φ^{-1}.

Let's take $k_1 = k_2 = 0$ (in other words, we are taking the solution with $x(0) = y(0) = 0$). The main job that remains is to do the integral. After the integral is done it will still have to be multiplied by Φ.

(i) Finish doing the integral. You will need trig identities for things like $\sin A \cos B$ and $\cos A \cos B$ to do them easily. Or I suppose you could have Desmos or WolframAlpha do it for you.

(ii) Your integral will have some stuff that has a prefactor of $\frac{1}{1-\omega}$ and other stuff that doesn't. Imagine that ω is very near resonance (e.g., very near 1). The terms with this prefactor will blow up and the others will be negligible. To simplify this part, in your final answer (which includes the factor of Φ out front of the integral), only include the terms that blow up for ω very near 1. To simplify, you will also be busting out your trig identities again.