

P3317 HW from Lecture 1 and Recitation 1

Due Tuesday September 4

Two atoms are walking down the street.

Atom 1: I think I lost an electron.

Atom 2: Are you sure?

Atom 1: Yes, I am positive.

Problem 1. Ion Detector An experimentalist drops helium ions onto a multichannel plate (this is like a digital camera that looks at ions instead of photons – look it up on Wikipedia – its actually a really cool application of quantum mechanics – they are also sensitive to UV photons, so they make night vision goggles from them). We will assume that the detector has 100% quantum efficiency (that means that whenever an ion hits it, one gets a count). We also will assume that it has no “dark current,” meaning that we never get a count if there are no ions hitting the detector. Usually these are two dimensional devices (like a camera).

Note: This is not a trick problem, it is supposed to be *easy*. If it does not seem easy, then you should ask for clarification.

1.1. Can this device simultaneously measure the x-position and the y-position of an ion? Explain how this is consistent with the idea that in quantum mechanics one cannot always measure two quantities simultaneously. What does this tell you about the commutation relationship between the x and y operators?

1.2. An ion hits the plate. At the time of contact, it has a wavefunction $\psi(x, y) = (1/\sqrt{2})(\phi_1(x, y) + \phi_2(x, y))$, where

$$\phi_1(x, y) = \begin{cases} \frac{1}{\sqrt{\pi d^2}} & \text{if } x^2 + y^2 < d^2 \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

$$\phi_2(x, y) = \begin{cases} \frac{1}{\sqrt{\pi d^2}} & \text{if } (x - a)^2 + y^2 < d^2 \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

Here $d = 1\mu\text{m}$, and $a = 1\text{mm}$. (a) Show that ψ is properly normalized. (b) How many counts will the microchannel plate detect? (c) Explain where the microchannel plate will say the ion is located.

Problem 2. Finite Differences in Time A very powerful technique (which we will explore at length in this course) is to treat space and time as discrete instead of continuous. An example we will explore at length in lecture 4 is the case of Ammonia (and if you want more details you can read the lecture notes). In ammonia, a Nitrogen atom has two locations in space where it can be.

To describe its quantum state, we just need to specify the amplitude for the atom to be in each of the locations: ψ_0 and ψ_1 , which you can think of as $\psi(r_0)$ and $\psi(r_1)$. The physical meaning of $|\psi_0|^2$ and $|\psi_1|^2$ are the probabilities that the particle is in each of the two locations. If you want to connect this with problem 1, you could imagine

$$\psi(x, y) = \begin{cases} \frac{\psi_0}{\sqrt{\pi d^2}} & \text{if } (x - x_0)^2 + (y - y_0)^2 < d^2 \\ \frac{\psi_1}{\sqrt{\pi d^2}} & \text{if } (x - x_1)^2 + (y - y_1)^2 < d^2 \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

The time dependent Schrodinger equation is a linear differential equation which is first order in time. In lecture 4 we will argue that the correct form for ammonia is

$$\begin{pmatrix} i\hbar\partial_t\psi_0(t) \\ i\hbar\partial_t\psi_1(t) \end{pmatrix} = \begin{pmatrix} A & B \\ B^* & D \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix} \quad (6)$$

where A, B, B^* , and D are parameters which define the Hamiltonian – B^* is the complex conjugate of B . For simplicity we will consider the case $A = D = 0$ and $B = -1$, and use units where $\hbar = 1$. As we will discuss, this is a good model for Ammonia. The coefficient B represents a *tunneling* process. It allows the particle to move from point r_0 to point r_1 and back.

In this problem we will solve this differential equation. This is pretty easy when we are dealing with 2×2 matrices, but for systems with more degrees of freedom it starts to become difficult. To help, we will introduce a general method for putting equations like this on a computer: the finite difference approximation. In particular, we will relate $\psi_0(t + \delta t)$ and $\psi_1(t + \delta t)$ to $\psi_0(t)$ and $\psi_1(t)$. In the next few homeworks we will investigate various different possible discretizations. We will find one of them, the “unitary semi-implicit method” to be better than the others. We will use this unitary finite difference approach in recitations 3 and 4.

2.1. Exact Solution

Solve the differential equations

$$i\psi_0'(t) = -\psi_1(t) \quad (7)$$

$$i\psi_1'(t) = -\psi_0(t) \quad (8)$$

with the initial conditions

$$\psi_0(0) = 1 \quad (9)$$

$$\psi_1(0) = 0. \quad (10)$$

You may find it easier to first eliminate ψ_1 , and write a second order differential equation for ψ_0 .

2.2. Deriving Forward Euler We will now consider an approximation to Eq. (7). We will turn this differential equation into a difference equation via Taylor’s theorem. Recall

$$f(t + \delta t) = f(t) + \delta t f'(t) + \frac{(\delta t)^2}{2!} f''(t) + \dots \quad (11)$$

If δt is small, we can truncate this at the second term, approximating

$$f(t + \delta t) \approx f(t) + \delta t f'(t), \quad (12)$$

or equivalently

$$f'(t) \approx \frac{f(t + \delta t) - f(t)}{\delta t}. \quad (13)$$

Taking $f = \psi_0$ and $f = \psi_1$, we can substitute this expression into EQ. (7) to get an equation of the form

$$\begin{pmatrix} \psi_0(t + \delta t) \\ \psi_1(t + \delta t) \end{pmatrix} = \mathbb{M} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix}, \quad (14)$$

where \mathbb{M} is a 2×2 matrix. Find \mathbb{M} .

2.3. Solving the Forward Euler Equations – the eigenvalue problem: From EQ. (14), one has

$$\begin{pmatrix} \psi_0(N\delta t) \\ \psi_1(N\delta t) \end{pmatrix} = \mathbb{M}^N \begin{pmatrix} \psi_0(0) \\ \psi_1(0) \end{pmatrix} \quad (15)$$

We would like to have a closed form expression for $\psi_0(N\delta t)$ and $\psi_1(N\delta t)$ when $\psi_0(0) = 1$ and $\psi_1(0) = 0$. [If we were doing this on a computer it would be trivial – we just do a bunch of matrix multiplications. Here, however, we want to do it by hand.]

There are several approaches to this sort of problem, but one classic approach starts with finding the eigenvalues λ, λ' and eigenvectors of \mathbb{M} :

$$\mathbb{M} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \lambda \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \quad (16)$$

and

$$\mathbb{M} \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = \lambda' \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}. \quad (17)$$

One then finds coefficients A and B such that

$$\begin{pmatrix} \psi_0(0) \\ \psi_1(0) \end{pmatrix} = A \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} + B \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}. \quad (18)$$

Matrices are *linear* operators, so

$$\mathbb{M}^n \begin{pmatrix} \psi_0(0) \\ \psi_1(0) \end{pmatrix} = A \mathbb{M}^n \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} + B \mathbb{M}^n \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}. \quad (19)$$

We can now use EQ. (16) and (17) to get

$$\mathbb{M}^n \begin{pmatrix} \psi_0(0) \\ \psi_1(0) \end{pmatrix} = A(\lambda)^n \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} + B(\lambda')^n \begin{pmatrix} b_0 \\ b_1 \end{pmatrix}. \quad (20)$$

Find $\lambda, \lambda', a_0, a_1, b_0, b_1$.

2.4. Find A and B .

2.5. Find $\psi_0(N\delta t)$ and $\psi_1(N\delta t)$.

2.6. **Comparison** We want to understand how good our approximation is. Use a computer to make a plot which has time on the horizontal axis, and $|\psi_0|^2$ on the vertical axis. Plot the exact result for $0 < t < 10\pi$. Also plot the result of the Forward Euler Approximation, using timesteps $\delta t = 0.1$ and $\delta t = 0.01$. Properly label the axes, and include a legend.

Problem 3. Gaussian Integrals

3.1. What is

$$\int_{-\infty}^{\infty} dx e^{-\alpha x^2} ? \quad (21)$$

No need to show your work.

3.2. What is

$$\int_{-\infty}^{\infty} dx e^{-\alpha(x-\frac{a}{2\alpha})^2} ? \quad (22)$$

No need to show your work. [Hint: x is a dummy variable.]

3.3. What is

$$\int_{-\infty}^{\infty} dx e^{-\alpha x^2 - ax} ? \quad (23)$$

No need to show your work. [Hint: You can calculate this in one or two lines from your results in 3.2]

3.4. Taylor expand your expression from Eq. (3.3) in powers of a about $a = 0$.

3.5. The integral in Eq. 23 can be written as

$$\int_{-\infty}^{\infty} dx e^{-\alpha x^2 - ax} = \sum_j \frac{a^j}{j!} \int_{-\infty}^{\infty} dx x^j e^{-\alpha x^2}. \quad (24)$$

By uniqueness of the Taylor expansion you can equate the coefficients of the powers of a in this expansion with the equivalent terms in 3.4. Use this equality to find

$$I_{2n} = \int_{-\infty}^{\infty} dx x^{2n} e^{-\alpha x^2}. \quad (25)$$

You may find it helpful to tattoo this answer on your fore-arm. You *will* use this again, and you do not want to have to derive it every time you use it.

Problem 4. Dirac delta function The Dirac delta function $\delta(x)$ is what the mathematicians refer to as a “distribution”. For them it is an object which really only makes sense inside an integral. We are physicists, though, so we will think of it as a function (or the limit of a function). The defining characteristic of the delta function is that for any function $f(x)$,

$$\int_a^b dx f(x)\delta(x) = f(0), \quad (26)$$

as long as $a < 0 < b$. Crudely, $\delta(x)$ is zero if $x \neq 0$ but is infinite when $x = 0$.

The simplest representation of the dirac delta function is as a limit of a “hat function”. We define

$$\delta_s(x) = \begin{cases} 1/s & -s/2 < x < s/2 \\ 0 & \text{otherwise} \end{cases} \quad (27)$$

We then define $\delta(x) = \lim_{s \rightarrow 0} \delta_s(x)$.

4.1. For any well behaved function $f(x)$, we can Taylor expand near $x = 0$, and write

$$f(x) = f_0 + f_1x + f_2x^2 + \dots \quad (28)$$

In terms of the coefficients of this Taylor series (keeping only up to second order) calculate

$$I_s = \int_{-\infty}^{\infty} dx f(x) \delta_s(x). \quad (29)$$

4.2. Find

$$\lim_{s \rightarrow 0} I_s. \quad (30)$$

4.3. In class I mentioned that the square of a delta function is poorly behaved. Calculate

$$J_s = \int_{-\infty}^{\infty} dx \delta_s(x)^2. \quad (31)$$

4.4. Find

$$\lim_{s \rightarrow 0} J_s. \quad (32)$$

4.5. There are a number of useful delta-function identities. By using a change of variables in the limit, show that for any positive number α ,

$$\delta(\alpha x) = \frac{\delta(x)}{\alpha}. \quad (33)$$

4.6. Another useful representation of the delta-function is as the limit of a Lorentzian:

$$\tilde{\delta}_s(x) = \frac{1}{\pi} \frac{s}{x^2 + s^2}. \quad (34)$$

We can define $\delta(x) = \lim_{s \rightarrow 0} \tilde{\delta}_s(x)$.

Make a properly labeled graph of $\tilde{\delta}_s(x)$, taking $s = 0.01$. Choose the axes range to show the relevant structure.

4.7. What is $\tilde{\delta}_s(x = 0)$?

4.8. At what value of x is $\tilde{\delta}_s(x) = \tilde{\delta}_s(0)/2$? From that result, give a reasonable expression for the “width” of $\tilde{\delta}_s(x)$.

4.9. From those results we see that $\tilde{\delta}_s(x)$ is sharply peaked about $x = 0$ – falling off on a length-scale of order s . If we take s sufficiently small, then any reasonable $f(x)$ will be roughly constant over this regime and

$$\tilde{I}_s = \int_{-\infty}^{\infty} dx f(x) \tilde{\delta}_s(x) \approx f(0) \int_{-\infty}^{\infty} dx \tilde{\delta}_s(x). \quad (35)$$

Evaluate this last integral to estimate \tilde{I}_s . Feel free to use integral tables or computerized algebra systems for doing these integrals.

4.10. Yet another common representation is

$$\bar{\delta}_s(x) = \frac{s \sin^2(x/s)}{\pi x^2}. \quad (36)$$

Make a properly labeled graph of $\bar{\delta}_s(x)$, taking $s = 0.01$. Choose the axes range to show the relevant structure.

4.11. Again, $\bar{\delta}_s(x)$ is sharply peaked about $x = 0$ – falling off on a length-scale of order s . If we take s sufficiently small, then $f(x)$ will be roughly constant over this regime and

$$\bar{I}_s = \int_{-\infty}^{\infty} dx f(x) \bar{\delta}_s(x) \approx f(0) \int_{-\infty}^{\infty} dx \bar{\delta}_s(x). \quad (37)$$

Evaluate this last integral to estimate \bar{I}_s . Feel free to use integral tables or computerized algebra systems for doing these integrals.

Problem 5. Feedback

5.1. How long did this homework take?

5.2. Which of the following words come to mind when you think about this homework (feel free to add your own words if you have something better): frustrating, fun, tedious, insightful, hard, easy, useful, useless, fair, unfair