MATH 231: CALCULUS II, HONORS PROJECT 01
INTRODUCTION TO THE SCHRÖDINGER EQUATION

Summary. Recall the time-independent Schrödinger equation

$$H\psi(x) = E\psi(x),$$

where H is the Hamiltonian of our system. For us, considering a particle in one dimension of mass m, we have

$$H\psi(x) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) + V(x)\psi(x).$$

In this worksheet, you will get some practice dealing with differential equations of this sort. As a first example, you will also solve the time-independent Schrödinger equation for a free particle, i.e., one subject to no potential. Along the way, you will use Heisenberg's uncertainty principle for position and momentum to asses the (non)physicality of your solution for the free particle.

Exercise 1 (First Steps)**.** For each of the following differential equations, find a function $f(x)$ that satisfies it.

(i) $\dfrac{\mathrm{d}}{\mathrm{d}x}f(x) = -f(x)$ Hint: Which function is its own derivative? Then figure out how to add the negative sign.

(ii) $\dfrac{\mathrm{d}^2}{\mathrm{d}x^2}f(x) = -f(x)$ Hint: Which functions have "cyclic" derivatives?

Solution.

(i)

(ii)

□

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Exercise 2 (Separation of Variables)**.** Letting $y = f(x)$, the first differential equation in the previous exercise can be rewritten as

$$\frac{\mathrm{d}y}{\mathrm{d}x} = -y.$$

Using the standard abuse of notation, we can treat $\mathrm{d}y \,/\, \mathrm{d}x$ as a fraction and multiply both sides by $\mathrm{d}x$:

$$\mathrm{d}y = -y \,\mathrm{d}x\,.$$

Dividing through by y gives us

$$\frac{1}{y}\,\mathrm{d}y = -\,\mathrm{d}x\,.$$

We have separated all the xs and ys, so we can integrate both sides to obtain

$$\begin{aligned}
\int \frac{1}{y}\,\mathrm{d}y &= \int -1\,\mathrm{d}x \\
\ln|y| + C_1 &= -x + C_2 \\
\ln|y| &= -x + C_2 - C_1 \\
e^{\ln|y|} &= e^{-x+C_2-C_1} \\
|y| &= e^{-x}(e^{C_2}e^{-C_1}).
\end{aligned}$$

Writing $C = \pm e^{C_2}e^{-C_1}$ for our constant of integration (with sign), we find

$$y = Ce^{-x}.$$

Note that we divided by y, so we should be careful to check that $y = 0$ is still included in our general solution. Of course, setting $C = 0$ does exactly that.

(i) Our second equation can be rewritten as

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}y}{\mathrm{d}x} = -y.$$

Let $z = \mathrm{d}y \,/\, \mathrm{d}x$. Use the chain rule to show

$$\frac{\mathrm{d}z}{\mathrm{d}x} = \frac{\mathrm{d}z}{\mathrm{d}y}z.$$

Conclude that our equation is the same as

$$\frac{\mathrm{d}z}{\mathrm{d}y}z = -y.$$

(ii) Use the separation of variables technique sketched above on this new equation from (i) to find that

$$z = \pm\sqrt{C^2 - y^2},$$

where C is some scaled constant of integration.

(iii) Since $z = \mathrm{d}y \,/\, \mathrm{d}x$, the previous part led us to a new differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \pm\sqrt{C^2 - y^2},$$

and separating gives

$$\frac{1}{\sqrt{C^2 - y^2}}\,\mathrm{d}y = \pm\,\mathrm{d}x\,.$$

Use a trigonometric substitution to obtain

$$\arcsin\left(\frac{y}{C}\right) = \pm x + D,$$

so that our general solution becomes

$$y = C\sin(\pm x + D).$$

Solution.

(i)

(ii)

(iii)

□

Remark 1 (Optional Algebra). Using some trigonometric identities, show that we can rewrite our expression for y in the previous exercise as

$$y = A\cos(x) + B\sin(x),$$

where $A = C\sin(D)$ and $B = C\cos(D)$.

Proof.

□

Exercise 3 (Free Particle)**.** Suppose our particle is moving in one dimension, but it is not being subjected to any potential. That is, $V(x) = 0$.

(i) Show that the time-independent Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) = E\psi(x).$$

(ii) Multiplying both sides of the above equation by $-2m/\hbar^2$, our differential equation becomes

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) = -\frac{2m}{\hbar^2}E\psi(x).$$

Assume E is real and positive, which we can write in the form $E = \lambda k^2$ for some $k > 0$. Use your solution to the previous exercise to guess (and explain) a solution

$$\psi(x) = A\cos(kx) + B\sin(kx),$$

where A and B are now allowed to be complex numbers.

(iii) Compute the second derivative

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) = \frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(A\cos(kx) + B\sin(kx)\right).$$

(iv) Use your computation in (iii) and the right-hand side of the differential equation in (ii) to determine an explicit formula for E. That is, find the real number λ. *(Hint: Your answer should involve $\hbar$ and m.)*

Solution.

(i)

(ii)

(iii)

(iv)

□

Exercise 4 (Nonphysicality)**.** By Euler's formula, we can rewrite our trigonometric solution $\psi(x)$ for the free particle as an exponential solution:

$$\psi(x) = Ce^{ikx} + De^{-ikx}.$$

Compute the squared $\mathcal{L}^2$-norm of the solution ψ from Exercise 3:

$$\|\psi\|_2^2 = \int_{-\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x \, .$$

Is ψ in our state space $\mathcal{L}^2$? *(Hint: Evaluate this like any other doubly infinite integral.)*

Solution.

□

Exercise 5 (Uncertainty)**.** Heuristically, Heisenberg's position-momentum uncertainty principle tells us that there is a *physical* limit to how precisely we can measure position and momentum simultaneously. Namely,

$$\sigma_x \sigma_p \geq \frac{\hbar}{2},$$

where σ_x and σ_p denote the standard deviations, i.e., the bigger the σ_x the more uncertain we are about position (and respectively for σ_p and momentum).[1] Note that if I know a particle's energy for certain, I also know (the magnitude of) its momentum. In this case, we are certain about momentum, so σ_p vanishes.

(i) In the previous exercise, we found a formula for E with certainty, so $\sigma_p = 0$. What "value" would σ_x have to take so that the uncertainty principle is satisfied?

(ii) In words, try to explain the connection between your answer to (i) and your solution to the previous exercise.

Solution.

(i)

(ii)

□

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[1] Later, during our investigation of expectation values, we will learn about standard deviations and give a proof of the uncertainty principle.