

Written report first draft

● Graded

Student

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Total Points

1 / 1 pts

Question 1

Completion

1 / 1 pt

✓ - 0 pts Correct

💬 This was great fun to read. I think you've got a good start (and your intro is excellent). You might want to narrow your scope a little bit, though. I'm not sure if it's really feasible to get through all of the examples in this amount of space (though I appreciate the enthusiasm!).

It's up to you, but it seems like you could cut down on the derivations of the Legendre/Hermite polynomials from your notes, and maybe don't include the 3d Schrödinger equation.

- 1 Good plan
- 2 Not sure how much you're planning to include, but you might want to think about cutting some of this down.
- 3 This is not a quantum mechanics class, so that's totally fair
- 4 What a flex (I cannot comment on these computations, but I'd imagine you've already thought about them a bit, so that should be fine)
- 5 Great setup.
- 6 I love this little history lesson

Outline

- Rough timing / spacing outline.
 - Intro to quantum mechanics (5 minutes / 750 words).
 - Using hypergeometric functions to mathematically solve the Hermite and Legendre equations (5 minutes / 750 words).
 - The complex analysis: Applications of residues to Rodrigues expressions, contour integrals and generating functions (8 minutes / 1200 words)
 - What the complex analysis indirectly gets you, e.g., certain physical properties like orthogonality and normalization that would be harder to compute directly (2 minutes / 300 words)

Intro to QMech Ideas

- A preview of where the complex analysis comes in.
 - This is an ordinary differential equation that physicists care about:
$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) \cdot \psi(x) = E\psi(x)$$
 - What do they do with it?
 - They take a potential energy function $V : \mathbb{R} \rightarrow \mathbb{R}$ of interest and use this equation to solve for a corresponding $\psi : \mathbb{R} \rightarrow \mathbb{R}$.
 - Some potential energy functions V give rise to special differential equations, such as the **Hermite equation** and **Legendre equation**.
 - Why do we care?
 - We can use complex analysis and the hypergeometric function introduced on Problem Set 2 to solve these equations and learn about their properties.
- Quantum mechanics background.
 - In the name of being concise in my background, I'm going to intentionally skip some details. You're free to ask me about these things, but I have done my best to present a cohesive, standalone introduction.
 - Quantum mechanics is better *done* than *understood* at first. Understanding typically develops with experience in doing the computations, which is a strange but fairly valid pedagogical approach. However, since I don't have the time to walk you through a bunch of computations, I will do my best to offer a handwavey verbal explanation.
 - Quote my physics textbook here??
 - Classical physics: Matter is composed of particles whose motion is governed by Newton's laws, most famously, the second-order differential equation

$$-\frac{dV}{dx} = F = ma = m \frac{d^2x}{dt^2}$$

- Analyze larger objects as collections of particles each evolving under Newton's laws.
- Matter has a fundamentally *particle-like* nature.
- New results challenge this postulate.
 - Einstein (1905): The photoelectric effect equation and the mass-energy equation.

$$E = h\nu = \frac{hc}{\lambda} \quad E = mc^2$$

- Combining these, we find that light has mass!

$$mc^2 = \frac{hc}{\lambda}$$

$$m = \frac{h}{\lambda c}$$

- Louis de Broglie (1924): Turns in a 4-page PhD thesis and says:

$$\lambda = \frac{h}{mc}$$

- Paris committee will fail him, but they write to Einstein who recognizes the importance of this work (Labalme, 2023, p. 7).
- Takeaway: de Broglie has just postulated that fundamental particles of matter (e.g., electrons) have a wavelike nature.
- Davisson-Germer experiment: Update to Thomas Young's double-slit experiment. They use electrons and *still* observe a diffraction pattern. Confirms de Broglie's hypothesis.

- So what is matter?
 - Modern physicists and chemists will say it has a **dual wave-particle nature**.
 - What does this mean? I mean, I can picture a wave, I can picture a particle, and they don't look the same! How should I picture it?
 - Remember, all we can do as scientists is provide a model to summarize our experimental results.
 - Occam's razor: Simpler models are better.
 - There are some experimental results in which light behaves like a particle and some in which it behaves like a wave. We will use each model when appropriate and leave the true nature of matter unsettled until we have more data.
- For the remainder of this discussion, let us confine ourselves to one-dimensional space.
- So if matter is a wave, then it is spread out over all space in some sense; it does not exist locally at some point x , but rather at each point $x \in \mathbb{R}$, it has some intensity $\psi(x)$ given by a wave function $\psi : \mathbb{R} \rightarrow \mathbb{R}$.
- What constraints can we put on ψ ?
- Schrödinger (1925):

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) \cdot \psi(x) = E\psi(x)$$

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- In the Swiss Alps with his mistress.
 - Wasn't just Oppenheimer.
- Richard Feynman: "Where did we get that [equation] from? Nowhere. It is not possible to derive it from anything you know. It came from the mind of Schrödinger."
- Feynman, true to character, was being mildly facetious, but the core of what he says is true: It was a pretty out-of-left-field result.
- So say we're given some potential $V(x)$ and get a $\psi(x)$ that solves the TISE. What does $\psi(x)$ tell us?
 - Nothing directly.
 - Born (1926): $|\psi(x)|^2$ gives the probability that the wave/particle is at x .
 - Examples likening densities to orbitals from Gen Chem I final review session..
- The universe can still be quantized even if we can't see it.
 - The Earth can still be round even if we can't see it.
 - The pixels in a screen can still be quantized even if we can't see them.

- Now, where is all of this going? Why am I talking about quantum mechanics in my complex analysis final project?

■ While you or I might care about the solutions to these questions in the abstract and just for funsies, the people who will pay you to do your research might not. As such, it is important to be able to explain to a non-mathematician where your problem comes from and how a solution will benefit the average Joe.

- This brings us to microwaves.

■ Personally, I like microwaves. They heat up food far more quickly than a traditional oven, they're energy efficient, and they go ding when they're done.

■ Microwaves work because of quantum mechanics.

■ Essentially, they shoot light of just the right frequency at your food so that molecules in it — which are already vibrating harmonically — vibrate faster. Faster vibrations means warmer food.

■ But how do we analyze such a vibrating molecule to know what frequency of light to shoot at it? Well, a vibrating molecule can be modeled as a quantum harmonic oscillator, that is, a quantum particle with

$$V(x) = \frac{1}{2}kx^2$$

■ Sparing you the gory details, if we plug this into the Schrödinger equation and do some rearranging, we end up having to solve the **Hermite equation**:

$$\frac{d^2H}{dy^2} - 2y\frac{dH}{dy} + (\epsilon - 1)H(y) = 0$$

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■ To solve the Hermite equation, we need complex analysis and the hypergeometric function.

- Alright, where else can we use such techniques?

■ What if we care about chemistry, at all?

■ Once atoms and molecules were discovered, chemistry developed as the discipline that uses atoms and molecules to do stuff, be it synthesizing a new medicine, mass-producing the ammonia fertilizer that feeds the planet, or literally anything else.

■ “Doing stuff” with atoms and molecules, however, is greatly facilitated by a good understanding of how atoms and molecules interact, and hence how they’re structured.

■ Once again, quantum mechanics provides the answers we need.

■ A classic example is the electronic structure of the hydrogen atom, which consists of a single electron (a quantum particle) existing in the potential

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

➢ FYI, that is not Euler’s number in the numerator but rather the charge of an electron.

■ Sparing you the gory details once again, if we plug this into the Schrödinger equation and do some rearranging, we end up having to solve the **Legendre equation**:

$$(1 - x^2)\frac{d^2P}{dx^2} - 2x\frac{dP}{dx} + \left[\ell(\ell + 1) - \frac{m^2}{1 - x^2}\right]P(x) = 0$$

- Labalme (2023, pp. 28–31): Hermite polynomials derivation.

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- Address the quantum harmonic oscillator.
 - Apply the 1D TISE.
 - Change coordinates.
 - Take an asymptotic solution.

- Discover that the general solutions are of the form $H(y)e^{-y^2/2}$.
- Substituting back into the TISE, we obtain the Hermite equation.
- Solve via a series expansion and recursion relation.
- Truncate the polynomial expansion to quantize.
- Labalme (2023, pp. 56–65): Legendre polynomials and associated Legendre functions derivation.
 - Address the hydrogen atom.
 - Starting from the 3D TISE in spherical coordinates, use separation of variables to isolate a one-variable portion of the angular equation. When rearranged, this ODE becomes **Legendre's equation**.
 - Solving Legendre's equation when $m = 0$ gives the Legendre polynomials $P_\ell(x)$.
 - Solving Legendre's equation when $m \neq 0$ gives the associated Legendre functions
- Labalme (2024, pp. 34–37): Much more detailed asymptotic analysis and derivation of the Hermite equation.
 - Here, we properly motivate the $H(y)e^{-y^2/2}$ that was just supplied last time.
 - Hermite polynomials are eventually defined via the following formula, which is *not* derived.
$$H_n(\xi) = (-1)^n \exp(\xi^2) \frac{d^n}{d\xi^n} [\exp(-\xi^2)]$$
- Labalme (2024, pp. 65–66): Legendre polynomials.
 - Labalme (2023) actually does a better job of deriving Legendre's equation and motivating why we need the associated Legendre functions.
 - The Legendre polynomials are given by Rodrigues' formula:
$$P_\ell(u) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{du^\ell} (u^2 - 1)^\ell$$
- The associated Legendre functions are defined as in Labalme (2023).

Applying Hypergeometric Functions Ideas

The Confluent Hypergeometric Equation

- In this section, Seaborn (1991) present a purposefully handwavey derivation of the confluent hypergeometric equation (and function) from the hypergeometric equation (and function). They do this so as to emphasize the connection between the two and their solutions and not get bogged down in the algebra. Let's begin.
- Define $x := bz$ in order to rewrite the hypergeometric function as follows.

$$\begin{aligned} F(a, b; c; z) &= \sum_{n=0}^{\infty} \frac{(a)_n (b+1) \cdots (b+n-1)}{n! (c)_n} z^n \\ &= \sum_{n=0}^{\infty} \frac{(a)_n (1 + \frac{1}{b}) \cdots (1 + \frac{n-1}{b})}{n! (c)_n} x^n \end{aligned}$$

- Taking the limit as $b \rightarrow \infty$ of the above yields the **confluent hypergeometric function**.

- **Confluent hypergeometric function:** The function defined as follows. *Denoted by ${}_1F_1$. Given by*

$${}_1F_1(a; c; x) := \sum_{n=0}^{\infty} \frac{(a)_n}{n!(c)_n} x^n$$

- Similarly, we may rewrite the hypergeometric equation using this substitution.

$$x \left(1 - \frac{x}{b}\right) \frac{d^2u}{dx^2} + \left[c - \left(\frac{a+1}{b} + 1\right)x\right] \frac{du}{dx} - au = 0$$

- Note that we have to use the chain rule when replacing the derivatives; this is how all the b 's work out. Essentially, we substitute $z = x/b$, $u(z) = u(x)$, $du/dz = b \cdot du/dx$, and $d^2u/dz^2 = b^2 \cdot d^2u/dx^2$; after that, we divide through once by b and simplify.
- Then once again, we take the limit as $b \rightarrow \infty$ to recover the **confluent hypergeometric equation**.

- **Confluent hypergeometric equation:** The differential equation given as follows, where $a, c \in \mathbb{C}$ are constants independent of x . *Given by*

$$x \frac{d^2u}{dx^2} + (c - x) \frac{du}{dx} - au = 0$$

- Let's investigate the singularities of the confluent hypergeometric equation and see how they stack up against the $0, 1, \infty$ of the hypergeometric equation.

- First off, observe that the confluent hypergeometric equation has singularities at $x = 0, \infty$.
- Rewriting the confluent hypergeometric equation in the standard form for a linear, second-order, homogeneous differential equation, we obtain

$$P(x) = \frac{c}{x} - 1 \quad Q(x) = -\frac{a}{x}$$

■ Since $xP(x) = c - x$ and $x^2Q(x) = -ax$ are both analytic at $x = 0$, the singularity at $x = 0$ is regular.

- How about the regularity of the singularity at $x = \infty$?

■ Change the variable to $y = x^{-1}$ and consider the resultant analogous singularity at $y = 0$.

■ This yields

$$\frac{d^2u}{dy^2} + \frac{y + (2 - c)y^2}{y^3} \frac{du}{dy} - \frac{a}{y^3} u = 0$$

■ Since $yP(y) = [1 + (2 - c)y]/y$ and $y^2Q(y) = -a/y$ — neither of which is analytic at $y = 0$ — the singularity at $x = \infty$ must be irregular.

■ In particular, this is because a merging (or **confluence**) of the singularities of the hypergeometric equation at $z = 1$ and $z = \infty$ has occurred.

- Finally, we will show that the confluent hypergeometric function constitutes a solution to the confluent hypergeometric equation and derive the general solution as well.

- Once again, we use the ansatz

$$u(x) = \sum_{k=0}^{\infty} a_k x^{k+s}$$

- Doing the casework and the recursion relation gets us to

$$u_1(x) = a_0 {}_1F_1(a; c; x) \quad u_2(x) = a_0 x^{1-c} {}_1F_1(1 + a - c; 2 - c; x)$$

so that if $c \notin \mathbb{Z}$, the general solution is

$$u(x) = A {}_1F_1(a; c; x) + B x^{1-c} {}_1F_1(1 + a - c; 2 - c; x)$$

One-Dimensional Harmonic Oscillator

- This is a prototypical sorted example of what kinds of strategizing I will do. Here, the math is heavier so that I can see exactly how it works. In a presentation, I'll be much more handwavey and with far fewer equations.
- The 1D quantum harmonic oscillator will now be solved using the methods developed in the previous section.
- The quantum mechanics.
 - Starting with the TDSE.
 - Separation of variables.
 - Solving the time component.
 - Arriving at the TISE.

$$\frac{d^2}{dx^2}u(x) + \left[\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}x^2 \right] u(x) = 0$$

- We will now go through several changes of variable to transform the above into the confluent hypergeometric equation.
 - To begin, we can clean up a lot of the constants via a change of independent variable $x = b\rho$.

■ Making this substitution yields

$$\begin{aligned} 0 &= \frac{1}{b^2} \frac{d^2}{d\rho^2} u(\rho) + \left[\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2} \cdot b^2 \rho^2 \right] u(\rho) \\ &= \frac{d^2}{d\rho^2} u(\rho) + \left[\frac{2mE}{\hbar^2} \cdot b^2 - \frac{m^2\omega^2}{\hbar^2} \cdot b^4 \rho^2 \right] u(\rho) \end{aligned}$$

■ Thus, if we define $b^4 = \hbar^2/m^2\omega^2$ (directly, this is $b := (\hbar/m\omega)^{1/2}$), we can entirely rid ourselves of the constants in front of the former $x^2u(x)$ term. This yields

$$0 = \frac{d^2}{d\rho^2} u(\rho) + \left[\frac{2E}{\hbar\omega} - \rho^2 \right] u(\rho)$$

■ Defining $\mu := 2E/\hbar\omega$ further cleans up the above, yielding

$$0 = \frac{d^2}{d\rho^2} u(\rho) + (\mu - \rho^2)u(\rho)$$

– Continuing to push forward, try the following substitution where h, g are to be determined.

$$u(\rho) = h(\rho)e^{g(\rho)}$$

■ The motivation for this change is that successive differentiations keep an $e^{g(\rho)}$ factor in each term that can be cancelled out to leave a zero-order term consisting of $f(\rho)$ multiplied by an arbitrary function of ρ . Choosing this latter function to be equal to the constant a from the confluent hypergeometric equation's zero-order term gives us a useful constraint. If this seems complicated, just watch the following computations.

■ Making the substitution, we obtain

$$\begin{aligned} 0 &= \frac{d^2}{d\rho^2} [he^g] + (\mu - \rho^2)he^g \\ &= \frac{d}{d\rho} [h'e^g + hg'e^g] + (\mu - \rho^2)he^g \\ &= [(h''e^g + h'g'e^g) + (h'g'e^g + hg''e^g + h(g')^2e^g)] + (\mu - \rho^2)he^g \\ &= [(h'' + h'g') + (h'g' + hg'' + h(g')^2)] + (\mu - \rho^2)h \\ &= h'' + 2g'h' + (\mu - \rho^2 + (g')^2 + g'')h \end{aligned}$$

- To make the zero-order term's factor constant, simply take $(g')^2 := \rho^2$. See how we've used the constancy constraint to define g ! Specifically, from here we get

$$\begin{aligned} g' &= \pm\rho \\ g &= \pm\frac{1}{2}\rho^2 \end{aligned}$$

- As to the sign question, we choose the sign that ensures $u(\rho) = h(\rho)e^{\pm\rho^2/2}$ does not blow up for large ρ . Naturally, this means that we choose the negative sign and obtain

$$u(\rho) = h(\rho)e^{-\rho^2/2}$$

- The differential equation also simplifies to the following under this definition of g .

$$0 = h'' - 2\rho h' + (\mu - 1)h$$

- One may recognize this as the Hermite equation!
- Through this $u(\rho)$ substitution method, we've effectively avoided the handwavey asymptotic analysis that physicists and chemists frequently use to justify deriving the Hermite equation.

- Alright, so this takes care of g ; now how about h ?
- To address h , we will need another independent variable change.
 - An independent variable change is desirable here because it can alter the first two terms without affecting the zero-order term.
 - Begin with the general modification $s := \alpha\rho^n$, where α, n are parameters to be determined.
 - Via the chain rule, the differential operators transform under this substitution into

$$\begin{aligned} \frac{d}{d\rho} &= \frac{ds}{d\rho} \cdot \frac{d}{ds} \\ &= n\alpha\rho^{n-1} \cdot \frac{d}{ds} \\ &= n\alpha(\alpha^{-1/n}s^{1/n})^{n-1} \cdot \frac{d}{ds} \\ &= n\alpha^{1/n}s^{1-1/n} \cdot \frac{d}{ds} \end{aligned}$$

and, without getting into the analogous gory details,

$$\frac{d^2}{d\rho^2} = n^2\alpha^{2/n}s^{2-2/n} \frac{d^2}{ds^2} + n(n-1)\alpha^{2/n}s^{1-2/n} \frac{d}{ds}$$

- Now another thing that the confluent hypergeometric equation tells us is that the second-order term needs an s in the coefficient. Thus, since $s^{2-2/n}$ is the current coefficient, we should choose $n = 2$ so that $s^{2-2/2} = s^1 = s$ is in the coefficient.
- This simplifies the operators to

$$\frac{d}{d\rho} = 2\alpha^{1/2}s^{1/2} \cdot \frac{d}{ds} \quad \frac{d^2}{d\rho^2} = 4\alpha s \frac{d^2}{ds^2} + 2\alpha \frac{d}{ds}$$

and hence the differential equation to

$$\begin{aligned} 0 &= 4\alpha s \frac{d^2h}{ds^2} + 2\alpha \frac{dh}{ds} - 2 \cdot \alpha^{-1/2}s^{1/2} \cdot 2\alpha^{1/2}s^{1/2} \cdot \frac{dh}{ds} + (\mu - 1)h(s) \\ &= 4\alpha s \frac{d^2h}{ds^2} + (2\alpha - 4s) \frac{dh}{ds} + (\mu - 1)h(s) \\ &= \alpha s \frac{d^2h}{ds^2} + \left(\frac{\alpha}{2} - s\right) \frac{dh}{ds} - \frac{1}{4}(1 - \mu)h(s) \end{aligned}$$

- Finally, to give the right coefficient in the second-order term and complete the transformation into the confluent hypergeometric equation, pick $\alpha = 1$.

$$0 = s \frac{d^2 h}{ds^2} + \left(\frac{1}{2} - s \right) \frac{dh}{ds} - \frac{1}{4}(1 - \mu)h(s)$$

- Now according to our prior general solution to the hypergeometric equation,

$$h(s) = A {}_1F_1\left(\frac{1}{4}(1 - \mu); \frac{1}{2}; s\right) + Bs^{1/2} {}_1F_1\left(1 + \frac{1}{4}(1 - \mu) - \frac{1}{2}; 2 - \frac{1}{2}; s\right)$$

- Under one last reverse change of variables back via $s = \rho^2$ and some simplification, we obtain

$$h(\rho) = A {}_1F_1\left(\frac{1}{4}(1 - \mu); \frac{1}{2}; \rho^2\right) + B\rho {}_1F_1\left(\frac{1}{4}(3 - \mu); \frac{3}{2}; \rho^2\right)$$

Boundary Conditions and Energy Eigenvalues

- Come back for more detail!!
- Under an asymptotic analysis, the confluent hypergeometric functions are diverging at large ρ .
- To prevent this, we need the series to terminate. By our previous results about series termination, this happens when either...
 1. $\frac{1}{4}(1 - \mu)$ is a nonpositive integer and $B = 0$;
 2. $\frac{1}{4}(3 - \mu)$ is a nonpositive integer and $A = 0$.
- The first case gives the even energy eigenvalues and Hermite polynomials, and the second case gives us the odd energy eigenvalues and Hermite polynomials.

Hermite Polynomials and the Confluent Hypergeometric Function

- Come back for more detail!!
- Formally defining the Hermite polynomials, and proving that they satisfy the Hermite equation.

Three-Dimensional Schrödinger Equation

- Very much analogously to Chapter 3, the hypergeometric function is used to tackle Legendre's equation, Legendre polynomials, and associated Legendre functions.
- Finally derives where $\ell(\ell + 1)$ comes from for the first time!

Complex Analysis Ideas

Legendre Polynomials

- Will get to use residue and the Γ function.
- Get to the Rodrigues formula.

Hermite Polynomials

- Rodrigues expression for the Hermite polynomials.

Tie-Back Ideas

- Chapter 10: Contour integral definitions of these two. Never seen in physics, but cool characterization!
- Chapter 11: Generating functions of these two. Same as above. Did Mazziotti allude to recursion relations??
- Mathematical applications of these to things I have seen, like normalization. How are these characterizations useful for proving certain physical properties, even if they're never discussed explicitly in intro courses?
- Applications to orthogonality relations: 12.4.

References

- Labalme, S. (2023). *CHEM 26100 (Quantum Mechanics) notes*. Retrieved May 10, 2024, from <https://github.com/shadypuck/CHEM26100Notes/blob/master/Notes/notes.pdf>
- Labalme, S. (2024). *PHYS 23410 (Quantum Mechanics I) notes*. Retrieved May 10, 2024, from <https://github.com/shadypuck/PHYS23410Notes/blob/master/Notes/notes.pdf>
- Seaborn, J. B. (1991). *Hypergeometric functions and their applications* [Texts in Applied Mathematics, No. 8]. Springer.