

MATH 27000 (Basic Complex Variables) Final Project Notes

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Part I

Preliminaries

1. What topic do you want to do your final project on?

Answer. Special differential equations in physics (Hermite, Bessel, Legendre, Laguerre, etc.) and hypergeometric functions. ☐

2. What will be the main reference(s) that you will base your project on?

Answer. Seaborn (1991). ☐

3. What is the main statement or question you want to address in your project? Be specific!

Answer. Where do the various formulas for the Hermite and Legendre polynomials come from? These two cases hold particular interest for me because of the time I've spent working with them in my quantum mechanics coursework without ever knowing where they come from. I'm very much a bottom-up learner, so I'm super excited to finally explore their origins from the simple to the complex, no pun intended. ☐

4. Everyone has to prove *something* in their project (it doesn't have to be the same as the main statement/question from above). What is one statement you will explain the proof of in your writeup?

Answer. The Cauchy residue theorem ☐

5. What complex analysis topic will go into the project?

Answer. Applications to converting the hypergeometric definition of the Legendre polynomials into Rodrigues's formula, which I saw last quarter but which came out of nowhere. ☐

6. Is there other background (not in the main reference) you will need to complete the project? If you don't have it, how will you go about learning it?

Answer. Not particularly. I know the quantum mechanics. I'm prepared for some misconceptions regarding functional analysis (e.g., orthogonal polynomials), but I trust I can address these as they arise and that my grasp of the "big picture" is good enough that I'll be able to concentrate on the details. ☐

References

- Fischer, W., & Lieb, I. (2012). *A course in complex analysis: From basic results to advanced topics* (J. Cannizzo, Trans.). Vieweg+Teubner Verlag.
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- 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.

Proposal Feedback

- 4/23:
- Excellent! I'll push you to focus on Hermite and Legendre, as a few other folks are thinking about special functions too, and this way you're all doing different topics.
 - Also, please please please, in your presentation do not assume that your audience knows the relevant quantum mechanics (you can in the writeup, even though I don't really).

Part II

Quantum Mechanics Review

CHEM 26100 Notes

5/10:

- 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.
- 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.

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

- 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):

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

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

- 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

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

➤ 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.
 - 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

$$P_\ell^{(m)}(x) = (1 - x^2)^{|m|/2} \frac{d^{|m|}}{dx^{|m|}} [P_\ell(x)]$$

PHYS 23410 Notes

- 5/10: • 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).

Part III

Textbook Notes

1 Special Functions in Applied Mathematics

1.1 Variables, Functions, Limits, and Continuity

5/10:

- Notes from the preface.
 - Instead of introducing special functions as solutions to an ODE of interest, we will define the special function in terms of the generalized hypergeometric series and then derive all its interesting properties from this definition.
 - We will not be simple, straightforward, or elegant; rather, we will furnish the clearest and most direct connections between the functions of applied math and the hypergeometric functions.
 - Prerequisites: Real analysis, general awareness of Schrödinger's equation. Intermediate physics courses will lend a greater appreciation for the book.
 - Mathematical topics are not introduced until needed (e.g., complex analysis doesn't come in until Chapters 7-8 with the exception of a few reminders along the way).
- Introduction to the chapter.
 - **Special function:** A mathematical function that occurs often enough in fields like physics and engineering to warrant special consideration, often expressed through extensive dedicated literature.
- Definition of **variable**, **function**, **single-valued** or **bijective** (function), **limit**, and **continuity**.

1.2 Why Study Special Functions?

- Sine is a special function!
 - Seaborn (1991) gives two completely different contexts in physics where it arises.

1.3 Special Functions and Power Series

- Special functions can be represented as a power series.
 - This is because “the behavior of a physical system is commonly represented by a differential equation” and “one very powerful method for solving differential equations is to assume a power series solution” (Seaborn, 1991, p. 3).
- As an example, Seaborn (1991) very neatly solves the classical harmonic oscillator in full generality using a power series solution!

1.4 The Gamma Function: Another Example from Physics

- **Gamma function:** The complex function defined as follows. *Denoted by $\Gamma(z)$. Given by*

$$\Gamma(z) := \int_0^{\infty} t^{z-1} e^{-t} dt$$

- Seaborn (1991) gives an example of $\Gamma(3/2)$ arising in the context of normalizing the Maxwell-Boltzmann distribution.

1.4.1 Properties of the Gamma Function

- By direct computation,

$$\Gamma(1) = 1$$

- Via integration by parts,

$$\Gamma(z + 1) = z\Gamma(z)$$

- Combining the last two, we have for all $n \in \mathbb{N}_0$,

$$\Gamma(n + 1) = n!$$

- Two alternative integral representations.

$$\frac{\Gamma(z + 1)}{a^{z+1}} = \int_0^\infty x^z e^{-ax} dx \qquad \Gamma(z) = \int_0^1 [\log(s^{-1})]^{z-1} ds$$

– Brief derivations given for these, as well as the following.

- Sum in the argument.

$$\Gamma(x + 1) = \int_0^\infty e^{-t} t^{x+y-1} dt$$

- Product.

$$\Gamma(x)\Gamma(y) = \Gamma(x + y) \int_0^\infty p^{x-1}(1-p)^{-x-y} dp$$

- If $y = 1 - x$ and $0 < x < 1$, then

$$\Gamma(x)\Gamma(1 - x) = \int_0^\infty \frac{p^{x-1}}{1+p} dp$$

- We have the specific value that

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

- **Duplication formula** (for Γ): The relation given as follows. *Given by*

$$\Gamma(z)\Gamma\left(z + \frac{1}{2}\right) = \sqrt{\pi} 2^{1-2z} \Gamma(2z)$$

1.4.2 Velocity Distribution in an Ideal Gas

- Seaborn (1991) finishes the derivation of the Maxwell-Boltzmann distribution using the properties in Section 1.4.1.

- **Incomplete gamma function:** The complex function defined as follows. *Denoted by $\gamma(z, b)$. Given by*

$$\gamma(z, b) := \int_0^b t^{z-1} e^{-t} dt$$

1.5 A Look Ahead

- Many techniques exist for evaluating definite integrals.
- Examples.
 - Contour integration (see Chapter 8).
 - $\Gamma\left(\frac{1}{2}\right)$ may be evaluated by this method; computation given in a later chapter.
 - Geometrical approach.
- **Elementary functions:** The mathematical functions like the sine, the cosine, and the exponential, along with polynomials and other algebraic expressions.
- We will focus on **higher transcendental functions**, of which Γ is one example.

2 Differential Equations and Special Functions

2.1 Infinite Series

- 5/10:
- If we're going to be extensively working with infinite series, we might as well review their properties.
 - Defines the n^{th} **partial sum**, **convergence**, **absolute** (convergence), and **uniform** (convergence).
 - Properties of uniformly convergent infinite series.
 1. $\{u_k\}$ continuous $\implies u$ continuous.
 2. $\{u_k\}$ continuous $\implies u$ integrable term by term.
 3. $\{u_k\} \subset C^1$ and $u'_k \rightarrow u'$ uniformly $\implies u$ differentiable term by term.
 - Assume that all of these properties hold for every series in Seaborn (1991) unless explicitly stated otherwise.

2.2 Analytic Functions

- **Real analytic** (function in (a, b)): A function f such that for each point $x_0 \in (a, b)$, $f(x)$ can be written as a power series

$$f(x) = \sum_{n=0}^{\infty} c_n (x - x_0)^n$$

where the numbers c_n are independent of x .

- The functions we encounter in physics and applied mathematics are generally analytic.
- The functions we encounter in this book certainly will be.
- Any function f that is analytic in the interval (a, b) may be represented by its **Taylor series** expanded about any point x_0 in the interval.
- **Radius of convergence.** Denoted by R .
- Seaborn (1991) motivates the **Pochhammer symbol** by using it to rewrite the Taylor series for $f(z) = (1 - z)^s$.
- **Pochhammer symbol:** The number defined inductively as follows, where $a \in \mathbb{C}$ and $n \in \mathbb{N}_0$. Denoted by $(a)_n$. Given by

$$\begin{aligned} (a)_0 &:= 1 \\ (a)_n &:= a(a+1)(a+2)(a+3) \cdots (a+n-1) \end{aligned} \quad (n = 1, 2, 3, \dots)$$

- Definition of the **geometric series**.
- Identities involving Pochhammer symbols.
 1. $n! = (n-m)!(n-m+1)_m$.
 2. $(c-m+1)_m = (-1)^m (-c)_m$.
 3. $(n+m)! = n!(n+1)_m$.
 4. $n! = m!(m+1)_{n-m}$.
 5. $(2n-2m)! = 2^{2n-2m} (n-m)! (\frac{1}{2})_{n-m}$.
 6. $(c)_{n+m} = (c)_n (c+n)_m$.
 7. $(c)_n = (-1)^m (c)_{n-m} (-c-n+1)_m$.
 8. $(c)_n = (-1)^{n-m} (c)_m (-c-n+1)_{n-m}$.
 9. $(-n)_{m-k} = (-n)_{m-n} (m-2n)_{n-k}$.

2.2.1 Series Expansion with Remainder

- **n^{th} remainder** (of f analytic): The difference between f and the first n terms of its Taylor series. Denoted by R_n . Given by

$$R_n(x) := f(x) - \sum_{k=0}^{n-1} \frac{f^{(k)}(a)}{k!} (x-a)^k$$

- Seaborn (1991) derives the Lagrange error bound.
 - He also provides an integral formula and works an example.

2.2.2 Integration of Infinite Series

- “Infinite series that converge uniformly can be integrated term by term” (Seaborn, 1991, p. 22).
- This allows us to find the Taylor series for certain functions.
 - Example: We already know the Taylor series for $(1+x^2)^{-1}$ by extrapolating from the geometric series, and this function is just the derivative of \tan^{-1} !

2.2.3 Inversion of Series

- Same as Section II.4 of Fischer and Lieb (2012), but with more terms given.

2.3 Linear Second-Order Differential Equations

- A clever method of solution for any linear, second-order, homogeneous differential equation.
 - Such equations can be written in the form

$$\frac{d^2}{dz^2}u(z) + P(z)\frac{d}{dz}u(z) + Q(z)u(z) = 0$$

- Rewrite the above as

$$u''(z) = f(z, u, u')$$

- Suppose u, u' are defined at z_0 .
- Then the above gives $u''(z_0)$.
- It follows by differentiating to

$$u^{(3)}(z) = \frac{df}{dz} = f'(z, u, u')$$

that $u^{(3)}$ can also be evaluated at z_0 .

- Assuming u is analytic, all higher derivatives of the above exist as well, so by evaluating these at z_0 and adding on the two given ones, we can construct the following Taylor series for u .

$$u(z) = \sum_{n=0}^{\infty} \frac{u^{(n)}(z_0)}{n!} (z - z_0)^n$$

- If this series has a nonzero radius of convergence, then the solution exists.

2.3.1 Singularities of a Differential Equation

- **Ordinary point** (of an ODE): A point z_0 for which $u(z_0), u'(z_0)$ can be assigned arbitrary values and the solution still exists.

– Example: In the harmonic oscillator, all times t_0 are ordinary points of the Newton's second law ODE because we can pick $x(t_0), x'(t_0) = v(t_0)$ arbitrarily and still solve the ODE for a trajectory.

- **Singular point** (of an ODE): A point z_0 for which $u(z_0), u'(z_0)$ cannot be assigned arbitrary values without the solution failing to exist somewhere. *Also known as singularity* (at z_0).

– Example: The ODE

$$z^2 u''(z) + azu'(z) + bu(z) = 0$$

has a singularity at 0. Indeed, if $u(0)$ has any value other than 0, the above equation will not hold unless either $u'(0)$ or $u''(0)$ are infinite.

- The above two definitions are often alternatively stated as follows: If both P, Q are analytic at z_0 , then z_0 is an ordinary point. Otherwise, the point is singular.

2.3.2 Singularities of a Function

- **Regular** (f at z_0): A point z_0 at which f is analytic.
- **Irregular** (f at z_0): A point z_0 at which f is not analytic.
- Definition of **pole** and **essential singularity**.

– In Chapter 7, we'll learn about **branch points**, an additional type of singularity.

2.3.3 Regular and Irregular Singularities of a Differential Equation

- **Regular** (singularity of an ODE): A singular point z_0 of an ODE for which $(z - z_0)P(z)$ and $(z - z_0)^2 Q(z)$ are analytic at z_0 .
- **Irregular** (singularity of an ODE): A singular point z_0 of an ODE that is not regular.

2.4 The Hypergeometric Function

- Definition of **rational** (function).
- All ODEs encountered in this book have at most three singularities.
 - A differential equation with at most three singularities has P, Q rational.
- A change of variables can convert such an ODE into Gauss's **hypergeometric equation**.
- **Hypergeometric equation**: The differential equation given as follows, where $a, b, c \in \mathbb{C}$ are constants independent of z . *Given by*

$$z(1-z)\frac{d^2u}{dz^2} + [c - (a+b+1)z]\frac{du}{dz} - abu = 0$$

– This ODE has its singularities at $0, 1, \infty$.

- Since every ODE we will encounter for the rest of the book can be transformed into the hypergeometric equation, we need only solve it once. After that, we can express solutions to other ODEs in terms of this solution.
- Solving the hypergeometric equation.

- Use the ansatz

$$u(z) = \sum_{n=0}^{\infty} a_n z^{n+s}$$

- Substituting in, collecting terms, and setting each coefficient equal to zero gives the recursion relations

$$s(s+c-1)a_0 = 0 \qquad a_{n+1} = \frac{(n+s)(n+s+a+b)+ab}{(n+s+1)(n+s+c)}a_n$$

- We now divide into cases ($a_0 = 0$, $s = 0$, and $s = 1 - c$).

- $a_0 = 0$: Implies that $a_n = 0$ for all n , and hence $u(z) = 0$ is the only solution.
- $s = 0$: The recursion relation simplifies to

$$a_{n+1} = \frac{(a+n)(b+n)}{(n+1)(c+n)}a_n$$

which yields the coefficients of the **hypergeometric function**.

- $s = 1 - c$: Discussed shortly.

- **Hypergeometric function**: The function defined as follows, which solves the hypergeometric equation in one case. Denoted by $F(a, b; c; z)$. Given by

$$F(a, b; c; z) := \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{n! (c)_n} z^n$$

2.4.1 Examples

- We have

$$\sum_{n=0}^{\infty} z^n = F(1, b; b; z) \qquad (1-z)^s = F(-s, b; b; z)$$

- Note that the left equation above is the geometric series!

2.4.2 Linearly Independent Solutions

- Miscellaneous observations, based on the form of the hypergeometric function.
 - If a or b is in $\mathbb{Z}_{\leq 0}$, then the series terminates (i.e., it is a polynomial).
 - The case where c is a negative integer or zero will be discussed shortly.
- Since the hypergeometric equation is a homogeneous, linear, second-order differential equation, its general solution is a linear combination of two **linearly independent** solutions u_1, u_2 .
- **Linearly independent** (functions): Two functions u_1, u_2 such that $c_1 u_1 + c_2 u_2 = 0$ iff $c_1 = c_2 = 0$.
- $u_1(z) = F(a, b; c; z)$ is one solution.
- The other one may be obtained as follows from the $s = 1 - c$ case.
 - Substituting in and rearranging the original recursion relation yields

$$\begin{aligned} a_{n+1} &= \frac{[n + (2 - c) - 1][n + (2 - c) - 1 + a + b] + ab}{[n + (2 - c)](n + 1)} a_n \\ &= \frac{(n + c' - 1 + a)(n + c' - 1 + b)}{(n + 1)(n + c')} a_n \\ &= \frac{(a' + n)(b' + n)}{(n + 1)(c' + n)} a_n \end{aligned}$$

- Thus, returning the substitutions,

$$u_2(z) = z^{1-c} F(1+a-c, 1+b-c; 2-c; z)$$

- Therefore, the general solution of the hypergeometric equation is

$$u(z) = AF(a, b; c; z) + Bz^{1-c} F(1+a-c, 1+b-c; 2-c; z)$$

2.4.3 If c is an Integer

- If $c = 1$, then $u_2(z)$ is not a new solution.
- If $c \geq 2$, then

$$(2-c)_k = (2-c)(3-c) \cdots (-1) \cdot 0 \cdot (-n+k+1)!$$

- Thus, the denominator vanishes in higher order terms and u_2 is not a valid solution.

- If $c \leq 0$, then

$$(c)_k = (-n)(-n+1) \cdots (-1) \cdot 0 \cdot (-n+k-1)!$$

- Similarly, the denominator vanishes in higher order terms and u_2 is not a valid solution.

- If $c \in \mathbb{Z}$ and a or b is an integer, too, then it may be possible to have solutions given by both series.
 - Example given.

2.5 The Simple Pendulum

- Seaborn (1991) uses the hypergeometric function and elliptic integrals to solve the simple pendulum of classical mechanics *exactly*, i.e., without resorting to the small angle approximation.
- Excellent to see! Come back to if I have time.

2.6 The Generalized Hypergeometric Function

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

$${}_pF_q(a_1, \dots, a_p; b_1, \dots, b_q; z) := \sum_{n=0}^{\infty} \frac{(a_1)_n \cdots (a_p)_n}{n! (b_1)_n \cdots (b_q)_n} z^n$$

2.7 Vandermonde's Theorem

- See AIMEPrep.pdf.
- **Vandermonde's theorem:** The following powerful relation useful in manipulating sums involving Pochhammer symbols. *Given by*

$$\sum_{m=0}^n \frac{(a)_m}{m!} \frac{(b)_{n-m}}{(n-m)!} = \frac{(a+b)_n}{n!}$$

Proof. Given. □

- Definition of the **Cauchy product**.

2.8 Leibniz's Theorem

- **Leibniz's theorem:** The following formula for the m^{th} derivative of the product of two analytic functions u, v . Given by

$$\frac{d^m}{dx^m}[u(x)v(x)] = \sum_{k=0}^m \frac{(m-k+1)_k}{k!} \left[\frac{d^k}{dx^k} u(x) \right] \left[\frac{d^{m-k}}{dx^{m-k}} v(x) \right]$$

Proof. Given; follows from Vandermonde's theorem. □

3 The Confluent Hypergeometric Function

3.1 The Confluent Hypergeometric Equation

5/10:

- 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.

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

– 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.

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

- 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 $d^2 u/dz^2 = b^2 \cdot d^2 u/dx^2$; 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

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

- 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

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

- Since $xP(x) = c - x$ and $x^2 Q(x) = -ax$ 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

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

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

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

3.2 One-Dimensional Harmonic Oscillator

- 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 to get

$$f(t) = f_0 e^{-iEt/\hbar}$$

- 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 $x^2 u(x)$ 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 and leaving out the ρ 's for clarity, 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 **Hermite's 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

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

and hence the differential equation to

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

- 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 confluent hypergeometric equation,

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

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

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

3.2.1 Boundary Conditions and Energy Eigenvalues

5/11:

- Quantum mechanics stipulates that when $|\rho|$ is large, $u(\rho)$ must not diverge.
 - This ensures that the wave function is normalizable.
- However, the current solutions do diverge at large $|\rho|$ in general. We can show this via the following asymptotic analysis.
 - We'll first investigate the leftmost confluent hypergeometric function in the above solution.
 - Using consecutive applications of the identity $\Gamma(z + 1) = z\Gamma(z)$, this function can be written in the form

$$\begin{aligned} {}_1F_1\left(\frac{1}{4}(1 - \mu); \frac{1}{2}; \rho^2\right) &= \sum_{k=0}^{\infty} \frac{\left(\frac{1}{4}(1 - \mu)\right)_k}{k! \left(\frac{1}{2}\right)_k} \rho^{2k} \\ &= \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1}{4}(1 - \mu)\right)} \sum_{k=0}^{\infty} \frac{\Gamma\left(k + \frac{1}{4}(1 - \mu)\right)}{k! \Gamma\left(k + \frac{1}{2}\right)} \rho^{2k} \end{aligned}$$

- As $k \rightarrow \infty$, we have $\Gamma\left(\frac{1}{4}(1 - \mu)\right) \rightarrow \Gamma\left(k + \frac{1}{2}\right) \rightarrow \Gamma(k)$. Hence, the terms come to be $\approx \rho^{2k}/k!$.

- Thus, by adding $\rho^{2k}/k!$ for small k and subtracting these terms off as well as the original terms for small k , we obtain the approximation

$${}_1F_1\left(\frac{1}{4}(1-\mu); \frac{1}{2}; \rho^2\right) \approx \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1}{4}(1-\mu)\right)} \left[\sum_{k=0}^{\infty} \frac{\rho^{2k}}{k!} - \text{polynomial in } \rho^2 \right]$$

- The first term above is the Taylor series for e^{ρ^2} , which will dominate at large $|\rho|$.
- Therefore, we have shown that at large $|\rho|$,

$${}_1F_1\left(\frac{1}{4}(1-\mu); \frac{1}{2}; \rho^2\right) \approx e^{\rho^2}$$

- By a symmetric argument, we find that at large $|\rho|$,

$${}_1F_1\left(\frac{1}{4}(3-\mu); \frac{3}{2}; \rho^2\right) \approx e^{\rho^2}$$

- Thus, at large $|\rho|$,

$$u(\rho) = h(\rho)e^{g(\rho)} = (\tilde{A}e^{\rho^2} + \tilde{B}\rho e^{\rho^2})e^{-\rho^2/2} = (\tilde{A} + \tilde{B}\rho)e^{\rho^2/2}$$

where \tilde{A}, \tilde{B} incorporate the other constants.

- To prevent this, we need the series to terminate. By our previous results about series termination (see Section 2.4.2), 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 $A = 0$.
- Note that we don't *always* need the other term to be zeroed out by its coefficient; however, doing it this way allows us to get the orthonormal basis of Hermite polynomials, and the other cases may be recovered as linear combinations of these polynomials.
- Continuing on, the first case gives the even energy eigenvalues and wave functions.
 - Let $-n/2$ be the nonpositive integer equal to $\frac{1}{4}(1-\mu)$.
 - Note that we write our nonpositive integer in this form in anticipation of future manipulations.
 - Then by the definition of μ ,

$$\begin{aligned} -\frac{n}{2} &= \frac{1}{4}(1-\mu) \\ \mu &= 1+2n \\ \frac{2E}{\hbar\omega} &= 1+2n \\ E_n = E &= \hbar\omega \left(n + \frac{1}{2}\right) \end{aligned} \quad (n = 0, 2, 4, \dots)$$

- Additionally,

$$u_n(\rho) = A_n {}_1F_1\left(-\frac{n}{2}; \frac{1}{2}; \rho^2\right) e^{-\rho^2/2}$$

- For even n , ${}_1F_1\left(-\frac{n}{2}; \frac{1}{2}; \rho^2\right)$ is a polynomial in even powers of ρ .

- The second case gives us the odd energy eigenvalues and wave functions.
 - Let $-(n-1)/2$ be the form of our nonpositive integer this time around.
 - Then by a similar argument,

$$E_n = E = \hbar\omega \left(n + \frac{1}{2}\right) \quad (n = 1, 3, 5, \dots)$$

- Similarly, once again,

$$u_n(\rho) = B_n \rho {}_1F_1\left(-\frac{1}{2}(n-1); \frac{3}{2}; \rho^2\right) e^{-\rho^2/2}$$

- For odd n , ${}_1F_1\left(-\frac{1}{2}(n-1); \frac{3}{2}; \rho^2\right)$ is a polynomial in odd powers of ρ .

3.2.2 Hermite Polynomials and the Confluent Hypergeometric Function

- We now rewrite the confluent hypergeometric series into more conventional forms.
- We will begin with $n \in 2\mathbb{N}$.
 - By the definition of the confluent hypergeometric function,

$${}_1F_1\left(-\frac{n}{2}; \frac{1}{2}; \rho^2\right) = \sum_{k=0}^{\infty} \frac{\left(-\frac{n}{2}\right)_k}{k! \left(\frac{1}{2}\right)_k} \rho^{2k}$$

- As discussed in Section 2.4.2, once k reaches $n/2 + 1$, the $\left(-\frac{n}{2}\right)_k$ term equals 0. Thus, we may notationally truncate the above series to

$${}_1F_1\left(-\frac{n}{2}; \frac{1}{2}; \rho^2\right) = \sum_{k=0}^{n/2} \frac{\left(-\frac{n}{2}\right)_k}{k! \left(\frac{1}{2}\right)_k} \rho^{2k}$$

- Additionally, to reorder the terms of the series from highest power to lowest power, change the summation index from k to $n/2 - k$.

$${}_1F_1\left(-\frac{n}{2}; \frac{1}{2}; \rho^2\right) = \sum_{k=0}^{n/2} \frac{\left(-\frac{n}{2}\right)_{n/2-k}}{\left(\frac{n}{2} - k\right)! \left(\frac{1}{2}\right)_{n/2-k}} \rho^{n-2k}$$

- Essentially, what we've done here is the following. For $n = 4$, the previous series would have output a Hermite polynomial like $12 - 48\xi^2 + 16\xi^4$. Now, the series will output $16\xi^4 - 48\xi^2 + 12$ because *it is counting down*.
- Of course, we need some more manipulations before this series will give actual Hermite polynomials, but this reversal demonstrates the idea.
- From here, we will invoke Pochhammer symbol identities 1, 2, and 5 from Section 2.2.
 - In particular, identities 1 and 2 are, respectively,

$$n! = (n - m)!(n - m + 1)_m \quad (c - m + 1)_m = (-1)^m(-c)_m$$

- Algebraically rearranging and combining these via transitivity, we obtain

$$\frac{c!}{(c - m)!} = (c - m + 1)_m = (-1)^m(-c)_m$$

and hence

$$(-c)_m = \frac{(-1)^{-m}c!}{(c - m)!} = \frac{(-1)^m c!}{(c - m)!}$$

- Making the substitutions $c := n/2$ and $m := n/2 - k$, we obtain

$$\left(-\frac{n}{2}\right)_{n/2-k} = \frac{(-1)^{n/2-k} \left(\frac{n}{2}\right)!}{\left[\frac{n}{2} - \left(\frac{n}{2} - k\right)\right]!} = \frac{(-1)^{n/2-k} \left(\frac{n}{2}\right)!}{k!}$$

- Additionally, identity 5 is

$$(2n - 2m)! = 2^{2n-2m} (n - m)! \left(\frac{1}{2}\right)_{n-m}$$

- Making the substitutions $n := n/2$ and $m := k$, we obtain

$$(n - 2k)! = 2^{n-2k} \left(\frac{n}{2} - k\right)! \left(\frac{1}{2}\right)_{n/2-k}$$

– Via these substitutions, it follows that

$$\begin{aligned}
 {}_1F_1\left(-\frac{n}{2}; \frac{1}{2}; \rho^2\right) &= \sum_{k=0}^{n/2} \frac{(-1)^{n/2-k} \left(\frac{n}{2}\right)! \cdot 2^{n-2k}}{k! \cdot (n-2k)!} \rho^{n-2k} \\
 &= (-1)^{n/2} \left(\frac{n}{2}\right)! \sum_{k=0}^{n/2} \frac{(-1)^{-k}}{k!(n-2k)!} (2\rho)^{n-2k} \\
 &= (-1)^{n/2} \left(\frac{n}{2}\right)! \sum_{k=0}^{n/2} \frac{(-1)^k}{k!(n-2k)!} (2\rho)^{n-2k} \\
 &= \frac{(-1)^{n/2} \left(\frac{n}{2}\right)!}{n!} \sum_{k=0}^{n/2} \frac{(-1)^k n!}{k!(n-2k)!} (2\rho)^{n-2k}
 \end{aligned}$$

- Via an analogous argument, if $n \in 2\mathbb{N} + 1$, then

$${}_1F_1\left(-\frac{1}{2}(n-1); \frac{3}{2}; \rho^2\right) = \frac{(-1)^{(n-1)/2} \left(\frac{1}{2}(n-1)\right)!}{2n!} \sum_{k=0}^{\frac{1}{2}(n-1)} \frac{(-1)^k n!}{k!(n-2k)!} (2\rho)^{n-2k}$$

- **Hermite polynomials:** The family of special functions defined as follows. *Denoted by $H_n(\rho)$. Given by*

$$H_n(\rho) = \frac{n!(-1)^{-n/2}}{\left(\frac{n}{2}\right)!} {}_1F_1\left(-\frac{n}{2}; \frac{1}{2}; \rho^2\right) \quad (n \text{ even})$$

$$H_n(\rho) = \frac{2n!(-1)^{(1-n)/2}}{\left(\frac{1}{2}(n-1)\right)!} {}_1F_1\left(-\frac{1}{2}(n-1); \frac{3}{2}; \rho^2\right) \quad (n \text{ odd})$$

– Via the normalization in this definition, we see that we can write the Hermite polynomials for *any* integer n as

$$H_n(\rho) = \sum_{k=0}^{[n/2]} \frac{(-1)^k n!}{k!(n-2k)!} (2\rho)^{n-2k}$$

where $[x]$ denotes the largest integer less than x .^[1]

- **Hermite's equation:** The linear, second-order, homogeneous differential equation whose solutions are the Hermite polynomials. *Given by*

$$H_n''(\rho) - 2\rho H_n'(\rho) + 2nH_n(\rho) = 0$$

- Note that $2n = \mu - 1$ since we have that $-\frac{n}{2} = \frac{1}{4}(1 - \mu)$ in the even case and $-\frac{1}{2}(n-1) = \frac{1}{4}(3 - \mu)$ in the odd case, both of which simplify to the equality in question.
- The Hermite polynomials qualify as solutions despite their constant coefficient because of the linearity of the solutions.
- The Hermite polynomials qualify as solutions despite their specific choice of a value because of the fact that the choice is simply a quantum-mechanical restriction to a subclass of mathematically broader solutions.

- Putting everything together, we may now write the harmonic oscillator eigenfunctions as

$$u_n(\rho) = N_n H_n(\rho) e^{-\rho^2/2}$$

where N_n is a normalization constant that will be determined in Chapter 12.

¹I.e., $[x]$ denotes the **floor function**.

5 The Central Force Problem in Quantum Mechanics

5.1 Three-Dimensional Schrödinger Equation

5/12:

- The hydrogen atom will now be solved using the methods developed previously.
- The quantum mechanics, summarized in Labalme (2023, pp. 56–58).
 - Starting with the 3D TISE.
 - Introduction of polar coordinates and a spherically symmetric potential.
 - The Laplacian in spherical coordinates.
 - Separation of variables into a radial and angular equation, with the separation constant being denoted λ so that, in particular,

$$\lambda = -\frac{1}{Y} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y$$

- The angular momentum operator.
- Separation of the angular variables into the polar and azimuthal equations, and solution to the azimuthal equation.
- This all gets us to one substitution — namely, $x = \cos \theta$ — away from a precursor to the general Legendre equation.

5.2 Legendre's Equation

- We have arrived at the following differential equation.

$$(1-x^2) \frac{d^2}{dx^2} f(x) - 2x \frac{d}{dx} f(x) + \left(\lambda - \frac{m^2}{1-x^2} \right) f(x) = 0$$

- This ODE has three regular singular points (at $x = \infty$ and $x = \pm 1$), so we will look to transform it into the typical hypergeometric equation.
- We now begin the changes of variable.
 - Begin with the (unmotivated) substitution

$$f(x) = v(x)w(x)$$

- Using this substitution and rewriting the resulting differential equation in terms of w yields

$$\begin{aligned} 0 &= (1-x^2) \frac{d^2}{dx^2} [vw] - 2x \frac{d}{dx} [vw] + \left(\lambda - \frac{m^2}{1-x^2} \right) vw \\ &= (1-x^2) \frac{d}{dx} [v'w + vw'] - 2x(v'w + vw') + \left(\lambda - \frac{m^2}{1-x^2} \right) vw \\ &= (1-x^2)[(v''w + v'w') + (v'w' + vw'')] - 2x(v'w + vw') + \left(\lambda - \frac{m^2}{1-x^2} \right) vw \\ &= (1-x^2)vw''(x) + [2(1-x^2)v' - 2xv]w'(x) + \left[(1-x^2)v'' - 2xv' + \left(\lambda - \frac{m^2}{1-x^2} \right) v \right] w(x) \end{aligned}$$

- For our next (unmotivated) substitution, we will let

$$v(x) = (1-x^2)^a$$

- To pin down the exact value of a , first observe that it would be nice if we could just divide the v out of the second-order term, leaving only an expression of the independent variable behind as in the hypergeometric equation's second term.
- However, doing this would also necessitate dividing v out of the rest of the equation. In particular, we would need the coefficient of the zero-order term to be constant following this division, i.e., we need the zero-order term as written to be proportional to v .^[2]
- Let c be the constant of proportionality.
- If $v = (1 - x^2)^a$, then

$$\begin{aligned} v'(x) &= a(1 - x^2)^{a-1} \cdot (-2x) \\ &= -2ax(1 - x^2)^{a-1} \end{aligned}$$

and

$$\begin{aligned} v''(x) &= -2a(1 - x^2)^{a-1} - 2ax(a-1)(1 - x^2)^{a-2} \cdot (-2x) \\ &= -2a(1 - x^2)^{a-1} + 4x^2(a^2 - a)(1 - x^2)^{a-2} \end{aligned}$$

- Substituting into the zero-order term's coefficient, we obtain

$$\begin{aligned} cv &= (1 - x^2) [-2a(1 - x^2)^{a-1} + 4x^2(a^2 - a)(1 - x^2)^{a-2}] \\ &\quad - 2x \cdot -2ax(1 - x^2)^{a-1} + \left(\lambda - \frac{m^2}{1 - x^2} \right) (1 - x^2)^a \\ c(1 - x^2)^a &= -2a(1 - x^2)^a + 4a^2x^2(1 - x^2)^{a-1} - 4ax^2(1 - x^2)^{a-1} \\ &\quad + 4ax^2(1 - x^2)^{a-1} + \lambda(1 - x^2)^a - m^2(1 - x^2)^{a-1} \\ c &= (\lambda - 2a) + (4a^2x^2 - m^2)(1 - x^2)^{-1} \end{aligned}$$

- Choosing a such that $4a^2 = m^2$ ensures that c is constant, since then

$$\begin{aligned} c &= \lambda - 2a + 4a^2(x^2 - 1)(1 - x^2)^{-1} \\ &= \lambda - 2a - 4a^2 \end{aligned}$$

- But if $4a^2 = m^2$, then $a = \pm|m|/2$ and hence

$$v(x) = (1 - x^2)^{\pm|m|/2}$$

- At this point, we have solved for the second-order coefficient $(1 - x^2)$ and the zero-order coefficient $(\lambda - 2a - 4a^2)$ of our transformed differential equation in terms of a . Let's look at the first-order coefficient now in terms of a .

- Using the above substitutions, this coefficient should be

$$\begin{aligned} \frac{1}{v} \cdot 2(1 - x^2)v' - 2xv &= \frac{2(1 - x^2) \cdot -2ax(1 - x^2)^{a-1} - 2x(1 - x^2)^a}{(1 - x^2)^a} \\ &= -2(1 + 2a)x \end{aligned}$$

- Now, let's put everything together for this second substitution.

- In terms of a , we get

$$(1 - x^2)w''(x) - 2(1 + 2a)xw'(x) - (4a^2 + 2a - \lambda)w(x) = 0$$

- Substituting $a = \pm|m|/2$, we get

$$(1 - x^2)w''(x) - 2(1 \pm |m|)xw'(x) - (m^2 \pm |m| - \lambda)w(x) = 0$$

²More thoughts on justifying this and the last claim?? See the comment on the zero-order factor being "proportional to v " on Seaborn (1991, pp. 72–73).

– Finally, we embark on our last substitution.

- The zero-order term is set at this point, so we just need to change the independent variable.
- In particular, looking at the second-order term, we would like to transform $1 - x^2$ into $z(1 - z)$. To facilitate this, let

$$1 - x^2 = \alpha z(1 - z)$$

where α is an undetermined constant.

- We can determine α using the following constraint.

$$\begin{aligned} z(1 - z) \frac{d^2 w}{dz^2} &= (1 - x^2) \frac{d^2 w}{dx^2} \\ &= \alpha z(1 - z) \left[\frac{d^2 w}{dz^2} \cdot \left(\frac{dz}{dx} \right)^2 + \frac{dw}{dz} \frac{d^2 z}{dx^2} \right] \\ \frac{1}{\alpha} \cdot \frac{d^2 w}{dz^2} + 0 \cdot \frac{dw}{dz} &= \left(\frac{dz}{dx} \right)^2 \cdot \frac{d^2 w}{dz^2} + \frac{d^2 z}{dx^2} \cdot \frac{dw}{dz} \end{aligned}$$

- Comparing like terms, the above constraint splits into the two constraints

$$\frac{1}{\alpha} = \left(\frac{dz}{dx} \right)^2 \qquad 0 = \frac{d^2 z}{dx^2}$$

- Using the right constraint above, we learn that there exist $a, b \in \mathbb{C}$ such that

$$z = ax + b$$

- Applying the left constraint above to this result tells us that

$$\alpha = \frac{1}{a^2}$$

- Thus, returning to the original equation,

$$\begin{aligned} 1 - x^2 &= \frac{1}{a^2} (ax + b) [1 - (ax + b)] \\ &= \frac{1}{a^2} (ax + b - a^2 x^2 - abx - abx - b^2) \\ 1 + 0x - x^2 &= \frac{1}{a^2} (b - b^2 + (a - 2ab)x - a^2 x^2) \\ 1 + 0x &= \frac{b - b^2}{a^2} + \frac{1 - 2b}{a} x \end{aligned}$$

- Comparing like terms, we obtain the two-variable two-equation system

$$1 = \frac{b - b^2}{a^2} \qquad 0 = \frac{1 - 2b}{a}$$

- Solving the right equation above, we learn that

$$b = \frac{1}{2}$$

- Using this to solve the left equation above, we learn that

$$\begin{aligned} 1 &= \frac{\frac{1}{2} - \frac{1}{4}}{a^2} \\ a &= \pm \frac{1}{2} \end{aligned}$$

- It follows that

$$\alpha = a^{-2} = 4$$

- The last remaining question is which sign we should choose for a . In fact, it doesn't matter, so WLOG we will choose the minus sign because it will simplify things later down the road.^[3]
- Therefore,

$$z = \frac{1}{2}(1 - x)$$

- Using this substitution, we obtain

$$\begin{aligned} 0 &= [1 - (1 - 2z)^2] \frac{d}{dz} \left(\frac{dw}{dz} \cdot -\frac{1}{2} \right) \cdot -\frac{1}{2} - 2(1 \pm |m|)(1 - 2z) \frac{dw}{dz} \cdot -\frac{1}{2} - (m^2 \pm |m| - \lambda)w(z) \\ &= \frac{1}{4}[1 - (1 - 4z + 4z^2)] \frac{d^2w}{dz^2} + (1 \pm |m| - 2z \mp 2|m|z) \frac{dw}{dz} - (m^2 \pm |m| - \lambda)w(z) \\ &= z(1 - z)w''(z) + [1 \pm |m| - 2(1 \pm |m|)z]w'(z) - (m^2 \pm |m| - \lambda)w(z) \end{aligned}$$

- We may now invoke our prior general solution to the hypergeometric equation.

- Observe that when $\theta = 0$,

$$z = \frac{1}{2}(1 - x) = \frac{1}{2}(1 - \cos \theta) = 0$$

- Since such points are physically *allowed*, we must discard the solution that is singular at $z = 0$ by setting $B = 0$ in the general solution.
- Therefore, the solution to the above differential equation that is fully acceptable on physical grounds is

$$w(z) = {}_2F_1(a, b; c; z)$$

where

$$a + b = 1 \pm 2|m| \qquad ab = m^2 \pm |m| - \lambda \qquad c = 1 \pm |m|$$

- Since the hypergeometric function is invariant under interchange of a, b , we may solve the left two equations above for a and b and WLOG take b to be the larger of the two. This yields

$$w(z) = {}_2F_1(\underbrace{\frac{1}{2}(1 - \sqrt{4\lambda + 1}) \pm |m|}_a, \underbrace{\frac{1}{2}(1 + \sqrt{4\lambda + 1}) \pm |m|}_b; \underbrace{1 \pm |m|}_c; z)$$

- To determine the right choice of sign, we examine the behavior of the complete solution at the physically accessible point $z = 0$ (equivalently, $x = 1$).
- Returning our substitutions, we obtain the following with a, b, c defined as above.

$$\begin{aligned} f(x) &= Av(x)w(x) \\ &= A(1 - x^2)^{\pm|m|/2} \sum_{k=0}^{\infty} \frac{(a)_k(b)_k}{k!(c)_k} [z(x)]^k \\ &= A(1 - x^2)^{\pm|m|/2} \left[1 + \sum_{k=1}^{\infty} \frac{(a)_k(b)_k}{k!(c)_k} \left(\frac{1}{2} - \frac{1}{2}x\right)^k \right] \end{aligned}$$

- As $x \rightarrow 1$, the quantity in brackets approaches 1 and $1 - x^2 \rightarrow 0$. Thus, to ensure that the $v(x)$ term does not become a pole (hence f stays well behaved near 1), we choose the positive sign.
- Recalling that the original instance of “ \pm ” in $v(x)$ is what led to all other instances, this one choice resolves all other sign choices.

³This appears to be what Seaborn (1991, p. 73) suggests with “will satisfy our requirements,” but am I reading this right??

- Therefore, the complete solution to the precursor to the general Legendre equation is

$$f(x) = A(1 - x^2)^{|m|/2} {}_2F_1\left(\frac{1}{2}(1 - \sqrt{4\lambda + 1}) + |m|, \frac{1}{2}(1 + \sqrt{4\lambda + 1}) + |m|; 1 + |m|; z\right)$$

- Finally, as with the Hermite polynomials, we can show that the series diverges at certain values of x , so we must put a termination condition on it.
- An example of a case where it currently diverges but should be physically accessible.
 - Consider the behavior of ${}_2F_1(a, b; c; z)$ at $z = 1$.
 - We have

$${}_2F_1(a, b; c; 1) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{k! (c)_k}$$

- This series diverges if there is ever a case in which the $(k + 1)^{\text{th}}$ term is not smaller than the k^{th} term.
 - In such a case, we would have

$$\frac{(a)_{k+1} (b)_{k+1}}{(k+1)! (c)_{k+1}} \geq \frac{(a)_k (b)_k}{k! (c)_k}$$

- This condition is equivalent to

$$\begin{aligned} (a + k)(b + k) &\geq (k + 1)(c + k) \\ ab + (a + b)k &\geq c + ck \end{aligned}$$

- Thus, in the limit of large k , this condition is fulfilled if $a + b \geq c$.
- Critically, in this particular case, $a + b$ actually *is* greater than c since $|m| \geq 0$:

$$\begin{aligned} a + b &= \left[\frac{1}{2}(1 - \sqrt{4\lambda + 1}) + |m|\right] + \left[\frac{1}{2}(1 + \sqrt{4\lambda + 1}) + |m|\right] \\ &= 1 + 2|m| \\ &\geq 1 + |m| \\ &= c \end{aligned}$$

- To address this divergence, we must require the series to terminate.
 - In particular, either a or b must be a nonpositive integer.
 - In fact, it is sufficient for a to be a nonpositive integer.

- This is because b nonpositive implies a nonpositive. Here's why.

Proof. Suppose b is a nonpositive integer. By choice, $b \geq a$. Since $a + b = 2|m| + 1$ is an odd natural number, we have that $a \neq b$ and hence the strict inequality $b > a$ holds. The $a + b = 2|m| + 1$ condition combined with the fact that $b \in \mathbb{Z}$ also implies that $a \in \mathbb{Z}$. Therefore, a is an integer strictly less than zero, as desired. \square

- In particular, a being a nonpositive integer means that

$$\frac{1}{2}(1 - \sqrt{4\lambda + 1}) + |m| = a = -n \quad (n = 0, 1, 2, \dots)$$

- Note: Since $a = -n$ and $a + b = 2|m| + 1$, it also follows that $b = n + 2|m| + 1$.

- This termination condition allows us to solve for λ .

$$\begin{aligned} -n &= \frac{1}{2}(1 - \sqrt{4\lambda + 1}) + |m| \\ -2(n + |m|) &= 1 - \sqrt{4\lambda + 1} \\ 4\lambda + 1 &= 1 + 4(n + |m|) + 4(n + |m|)^2 \\ \lambda &= (n + |m|)(n + |m| + 1) \end{aligned}$$

- Define $\ell := n + |m|$. Then the separation constant is

$$\lambda = \ell(\ell + 1) \quad (\ell = 0, 1, 2, \dots)$$

- Seaborn (1991) comments a bit on the physical interpretation of this quantization as quantized angular momentum.
- Additional consequence: Rearranging the definition of ℓ to $\ell - |m| = n \geq 0$, we obtain the following two relations between ℓ, m .

$$\ell \geq |m| \quad -\ell \leq m \leq \ell$$

- It follows that in terms of these new parameters, the solution to the precursor to the general Legendre equation is

$$f_{\ell m}(x) = A_{\ell m}(1 - x^2)^{|m|/2} {}_2F_1(-\ell + |m|, \ell + |m| + 1; |m| + 1; \tfrac{1}{2} - \tfrac{1}{2}x)$$

- **Legendre's equation:** The linear, second-order, homogeneous differential equation (with rational coefficients) given as follows, which is the special case of the precursor to the general Legendre equation obtained when $m = 0$ and $\lambda = \ell(\ell + 1)$. *Given by*

$$(1 - x^2)f''(x) - 2xf'(x) + \ell(\ell + 1)f(x) = 0$$

5.3 Legendre Polynomials and Associated Legendre Functions

- **Legendre polynomial** (of order ℓ): A solution to Legendre's equation. *Denoted by $P_\ell(x)$. Given by*

$$P_\ell(x) := {}_2F_1(-\ell, \ell + 1; 1; \tfrac{1}{2} - \tfrac{1}{2}x)$$

- **General Legendre equation:** The generalization of Legendre's equation that we originally solved above. *Given by*

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

- We now derive the **associated Legendre functions**.

- Differentiate p times the Legendre polynomial of order ℓ :

$$\frac{d^p}{dx^p}P_\ell(x) = (-1)^p \sum_{k=p}^{\infty} \frac{(-\ell)_k(\ell + 1)_k}{2^k k! (1)_k} (k - p + 1)_p (1 - x)^{k-p}$$

- Reindex $k - p$ to k :

$$\frac{d^p}{dx^p}P_\ell(x) = (-1)^p \sum_{k=0}^{\infty} \frac{(-\ell)_{k+p}(\ell + 1)_{k+p}}{2^{k+p} (k + p)! (1)_{k+p}} (k + 1)_p (1 - x)^k$$

- Iteratively apply Pochhammer symbol identity 6 from Section 2.2:

$$\begin{aligned} \frac{d^p}{dx^p}P_\ell(x) &= (-1)^p \sum_{k=0}^{\infty} \frac{(-\ell)_p(-\ell + p)_k(\ell + 1)_p(\ell + 1 + p)_k}{2^k 2^p (k + p)! (1)_p (1 + p)_k} (k + 1)_p (1 - x)^k \\ &= (-1)^p \frac{(-\ell)_p(\ell + 1)_p}{2^p (1)_p} \sum_{k=0}^{\infty} \frac{(-\ell + p)_k(k + 1)_p(\ell + 1 + p)_k}{2^k (k + p)! (1 + p)_k} (1 - x)^k \\ &= (-1)^p \frac{(-\ell)_p(\ell + 1)_p}{2^p p!} \sum_{k=0}^{\infty} \frac{(-\ell + p)_k(k + 1)_p(\ell + p + 1)_k}{2^k k! (k + 1)_p (p + 1)_k} (1 - x)^k \\ &= (-1)^p \frac{(-\ell)_p(\ell + 1)_p}{2^p p!} \sum_{k=0}^{\infty} \frac{(-\ell + p)_k(\ell + p + 1)_k}{2^k k! (p + 1)_k} (1 - x)^k \end{aligned}$$

- Use the hypergeometric function to simplify the notation above.

$$\frac{d^p}{dx^p} P_\ell(x) = (-1)^p \frac{(-\ell)_p (\ell+1)_p}{2^p p!} {}_2F_1(-\ell+p, \ell+p+1; p+1; \tfrac{1}{2} - \tfrac{1}{2}x)$$

- By relating $p \sim |m|$ and comparing the above to $f_{\ell m}(x)$, we can see that the functions defined as follows will be solutions to the general Legendre equation. Note that the big constant above takes the role of $A_{\ell m}$.

- **Associated Legendre functions:** The canonical solutions to the general Legendre equation. Also known as **associated Legendre polynomials**. Denoted by $P_\ell^m(x)$. Given by

$$P_\ell^m(x) := (1-x^2)^{|m|/2} \frac{d^{|m|}}{dx^{|m|}} P_\ell(x)$$

- Let's take an additional moment to relate the above definition to the preceding derivation.
 - Via the Pochhammer symbol identities from Section 2.2, we may obtain the identities

$$(-1)^{|m|} (-\ell)_{|m|} = (\ell - |m| + 1)_{|m|} \quad \text{Identity 2}$$

$$= \frac{\ell!}{(\ell - |m|)!} \quad \text{Identity 2}$$

and

$$(\ell + 1)_{|m|} = \frac{(\ell + |m|)!}{\ell!} \quad \text{Identity 3}$$

■ Note that $\ell - |m|$ is nonnegative and hence a valid argument for the factorial because $\ell \geq |m|$.

- Therefore,

$$\begin{aligned} P_\ell^m(x) &= (1-x^2)^{|m|/2} \frac{(-1)^{|m|} (-\ell)_{|m|} \cdot (\ell+1)_{|m|}}{2^{|m|} |m|!} {}_2F_1(-\ell+|m|, \ell+|m|+1; |m|+1; \tfrac{1}{2} - \tfrac{1}{2}x) \\ &= (1-x^2)^{|m|/2} \frac{\ell! \cdot (\ell+|m|)!}{2^{|m|} |m|! (\ell-|m|)! \cdot \ell!} {}_2F_1(-\ell+|m|, \ell+|m|+1; |m|+1; \tfrac{1}{2} - \tfrac{1}{2}x) \\ &= \frac{(\ell+|m|)! (1-x^2)^{|m|/2}}{2^{|m|} |m|! (\ell-|m|)!} {}_2F_1(-\ell+|m|, \ell+|m|+1; |m|+1; \tfrac{1}{2} - \tfrac{1}{2}x) \end{aligned}$$

- We now define an inner product on the Legendre polynomials to discuss their **orthogonality**.
 - Orthogonality will be covered more in Chapter 12 (including for associated Legendre functions!), but for now we will just say that by “ $P_\ell(x)$ is orthogonal to $P_{\ell'}(x)$ for $\ell \neq \ell'$,” we mean that

$$\int_{-1}^1 P_\ell(x) P_{\ell'}(x) dx = 0 \quad (\ell \neq \ell')$$

- We now prove this orthogonality relation.

Proof. Let $\ell \neq \ell'$. Since $P_\ell(x), P_{\ell'}(x)$ are both Legendre polynomials, they satisfy Legendre's equation. Mathematically, we have that

$$(1-x^2)P_\ell''(x) - 2xP_\ell'(x) + \ell(\ell+1)P_\ell(x) = 0$$

and

$$(1-x^2)P_{\ell'}''(x) - 2xP_{\ell'}'(x) + \ell'(\ell'+1)P_{\ell'}(x) = 0$$

Multiply the top equation above by $P_{\ell'}(x)$, the bottom by $P_\ell(x)$, and subtract the first from the second to obtain

$$(1-x^2)[P_\ell P_{\ell'}'' - P_{\ell'} P_\ell''] - 2x[P_\ell P_{\ell'}' - P_{\ell'} P_\ell'] + [\ell'(\ell'+1) - \ell(\ell+1)]P_\ell P_{\ell'} = 0$$

Using a bit of calculus, the left two terms above can be combined. Additionally, the rightmost term can be moved over to the right side of the equation. This yields

$$\frac{d}{dx}\{(1-x^2)[P_\ell P'_{\ell'} - P'_\ell P_{\ell'}]\} = [\ell(\ell+1) - \ell'(\ell'+1)]P_\ell P_{\ell'}$$

Integrating both sides from -1 to 1 yields

$$\begin{aligned} \int_{-1}^1 d(1-x^2)[P_\ell P'_{\ell'} - P'_\ell P_{\ell'}] &= \int_{-1}^1 [\ell(\ell+1) - \ell'(\ell'+1)]P_\ell P_{\ell'} dx \\ (1-x^2)[P_\ell(x)P'_{\ell'}(x) - P'_\ell(x)P_{\ell'}(x)] \Big|_{-1}^1 &= [\ell(\ell+1) - \ell'(\ell'+1)] \int_{-1}^1 P_\ell(x)P_{\ell'}(x) dx \end{aligned}$$

Since $1-x^2$ goes to 0 at both 1 and -1 , the left side of the above equation is zero. Thus, we can divide out the constant term in front of the integral on the right side of the above equation, leaving us with

$$0 = \int_{-1}^1 P_\ell(x)P_{\ell'}(x) dx$$

as desired. □

7 Complex Analysis

7.1 Complex Numbers

- 5/10:
- Starts off with a bunch of review, but gets into some more advanced stuff (and new topics like cut lines) that I should probably look into.

8 Applications of Contour Integrals

8.1 The Cauchy Residue Theorem

- 5/10:
- Largely review, but probably good to skim through in more depth.
 - Plus, I will need their proof of the Residue Theorem!!

9 Alternate Forms for Special Functions

9.3 Legendre Polynomials

- 5/10:
- Will get to use residue and the Γ function.
 - Get to the Rodrigues formula.
 - Elaborate on complex analytic topics like the Γ function.

9.4 Hermite Polynomials

- Rodrigues expression for the Hermite polynomials.

10 Integral Representations of Special Functions

10.4 Legendre Polynomials

- 5/10: • Contour integral definitions of these two. Never seen in physics, but cool characterization!

10.6 Hermite Polynomials

-

11 Generating Functions and Recursion Formulas

11.1 Hermite Polynomials

- 5/10: • Generating functions of these two. Same as above. Did Mazziotti allude to recursion relations??

11.4 Legendre Polynomials

-

12 Orthogonal Functions

12.4 Orthogonality and Normalization of Special Functions

- 5/10:
- 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.

Part IV

Final Report

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.

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

- 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):

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

- 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**:

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

- 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

$$V(r) = -\frac{e^2}{4\pi\epsilon_0 r}$$

➤ 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.

- 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

$$P_\ell^{(m)}(x) = (1-x^2)^{|m|/2} \frac{d^{|m|}}{dx^{|m|}} [P_\ell(x)]$$

- 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.

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

- 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.

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

- 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 $d^2 u/dz^2 = b^2 \cdot d^2 u/dx^2$; 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

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

- 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

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

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

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

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 $x^2 u(x)$ 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

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

and hence the differential equation to

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

- 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.

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