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 $b \to \infty$ of the above yields the **confluent hypergeometric function**.
- **Confluent hypergeometric function**: The function defined as follows. *Denoted by* $\boldsymbol{{}_1F_1}$. *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.

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

  - 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 $z = x/b$, $u(z) = u(x)$, $\mathrm{d}u/\mathrm{d}z = b \cdot \mathrm{d}u/\mathrm{d}x$, and $\mathrm{d}^2u/\mathrm{d}z^2 = b^2 \cdot \mathrm{d}^2u/\mathrm{d}x^2$; after that, we divide through once by b and simplify.
  - Then once again, we take the limit as $b \to \infty$ 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*

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

- 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

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

    - 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
$$\frac{\mathrm{d}^2u}{\mathrm{d}y^2}+\frac{y+(2-c)y^2}{y^3}\frac{\mathrm{d}u}{\mathrm{d}y}-\frac{a}{y^3}u=0$$
- 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
$$u(x)=\sum_{k=0}^{\infty}a_kx^{k+s}$$
  - Doing the casework and the recursion relation gets us to
$$u_1(x)=a_0\,{}_1F_1(a;c;x)\qquad\qquad u_2(x)=a_0x^{1-c}\,{}_1F_1(1+a-c;2-c;x)$$
so that if $c\notin\mathbb{Z}$, the general solution is
$$u(x)=A\,{}_1F_1(a;c;x)+Bx^{1-c}\,{}_1F_1(1+a-c;2-c;x)$$

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

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

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

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

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

- The motivation for this change is that successive differentiations keep an $\mathrm{e}^{g(\rho)}$ 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

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

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

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

- 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

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

and, without getting into the analogous gory details,

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

- 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

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

and hence the differential equation to

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

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

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

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

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

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

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

3.2.1 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.

3.2.2 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.