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 to get
$$f(t)=f_0\mathrm{e}^{-iEt/\hbar}$$
  - 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 and leaving out the ρ's for clarity, 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 **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

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

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 confluent 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

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

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

    - As $k\to\infty$, we have $\Gamma\left(\frac{1}{4}(1-\mu)\right)\to\Gamma\left(k+\frac{1}{2}\right)\to\Gamma(k)$. 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

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

- 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 $|\rho|$,

$$ {}_1F_1(\tfrac{1}{4}(1-\mu);\tfrac{1}{2};\rho^2) \approx \mathrm{e}^{\rho^2} $$

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

$$ {}_1F_1(\tfrac{1}{4}(3-\mu);\tfrac{3}{2};\rho^2) \approx \mathrm{e}^{\rho^2} $$

– Thus, at large $|\rho|$,

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

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,

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

– Additionally,

$$ u_n(\rho) = A_n\,{}_1F_1(-\tfrac{n}{2};\tfrac{1}{2};\rho^2)\mathrm{e}^{-\rho^2/2} $$

- For even n, ${}_1F_1(-\frac{n}{2};\frac{1}{2};\rho^2)$ 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,

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

– Similarly, once again,

$$ u_n(\rho) = B_n\rho\,{}_1F_1(-\tfrac{1}{2}(n-1);\tfrac{3}{2};\rho^2)\mathrm{e}^{-\rho^2/2} $$

- For odd n, ${}_1F_1(-\frac{1}{2}(n-1);\frac{3}{2};\rho^2)$ 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,
$$ {}_1F_1(-\tfrac{n}{2}; \tfrac{1}{2}; \rho^2) = \sum_{k=0}^{\infty} \frac{\left(-\frac{n}{2}\right)_k}{k! \left(\frac{1}{2}\right)_k} \rho^{2k} $$
  - 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
$$ {}_1F_1(-\tfrac{n}{2}; \tfrac{1}{2}; \rho^2) = \sum_{k=0}^{n/2} \frac{\left(-\frac{n}{2}\right)_k}{k! \left(\frac{1}{2}\right)_k} \rho^{2k} $$
  - Additionally, to reorder the terms of the series from highest power to lowest power, change the summation index from k to $n/2-k$.
$$ {}_1F_1(-\tfrac{n}{2}; \tfrac{1}{2}; \rho^2) = \sum_{k=0}^{n/2} \frac{\left(-\frac{n}{2}\right)_{n/2-k}}{\left(\frac{n}{2}-k\right)! \left(\frac{1}{2}\right)_{n/2-k}} \rho^{n-2k} $$
    - 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,
$$ n! = (n-m)!(n-m+1)_m \qquad\qquad (c-m+1)_m = (-1)^m(-c)_m $$
      - 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
$$ \left(-\tfrac{n}{2}\right)_{n/2-k} = \frac{(-1)^{n/2-k}\left(\frac{n}{2}\right)!}{\left[\frac{n}{2}-\left(\frac{n}{2}-k\right)\right]!} = \frac{(-1)^{n/2-k}\left(\frac{n}{2}\right)!}{k!} $$
    - Additionally, identity 5 is
$$ (2n-2m)! = 2^{2n-2m}(n-m)!\left(\tfrac{1}{2}\right)_{n-m} $$
      - Making the substitutions $n := n/2$ and $m := k$, we obtain
$$ (n-2k)! = 2^{n-2k}\left(\tfrac{n}{2}-k\right)!\left(\tfrac{1}{2}\right)_{n/2-k} $$

- Via these substitutions, it follows that

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

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

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

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

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

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

  - 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

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

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

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