A discussion of particles in triangular potential wells and the quantum harmonic oscillator

Using power series to solve homogeneous, second-order ordinary differential equations with variable coefficients

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Abstract

This paper introduces the idea of solving differential equations by assuming a power series form for the solution. This method is briefly illustrated with an example, and then is used to solve both the Airy equation and the Hermite equation. The importance of these particular differential equations in quantum mechanics, more specifically triangular quantum wells and the quantum oscillator, is explored in detail, along with the real-life applications of these systems.

Contents

1 Personal section

My first real encounters with physics were in Year 9 (the United Kingdom equivalent of 8th grade). It was here that my passion for the subject was sparked, thanks to my teacher at the time: Mr. Andrew Brittain. His immense enthusiasm rubbed off on me. Two of his lessons, in particular, are imprinted in my memory. One was devoted entirely to particle physics and in the second, he discussed quantum tunnelling. Both these topics were well beyond our curriculum, but he thought that they would be of interest and serve as a valuable reminder that there was more to physics than studying changes of state or rolling a ball down a ramp. I remember being instantly captivated by the mystical world of quarks, and intrigued that it was, in fact, possible (though extremely unlikely) to run through a wall and appear on the other side!

Apart from physics, maths is another subject I enjoy. From a young age, I was drawn to the exactness and lack of ambiguity that maths offered. Over the years, I have taken part in several maths challenges, starting with the Primary Maths Challenge all the way to the Senior Maths Challenge just this year. I qualified for a number of follow-on rounds and olympiads along the way, all of which really stimulated my mind and helped me to think outside the box.

My experience of maths was completely transformed, however, when I began to teach myself calculus last summer. In a matter of days, all of the mesmerising symbols and equations I had seen in books and websites became something I could actually understand and use. A whole new world opened up before me. I started small, beginning with the rules for differentiation. Once I felt like I had mastered them, I moved onto integration, and was struck by the difference between the two types of calculus. Whilst differential calculus is a process, integral calculus is more of an art. After learning the basic methods of solving integrals, I started to add more interesting techniques, such as differentiating under the integral sign (the Leibniz method) and the Ostogradsky method of integration, to my repertoire. Before I knew it, solving integrals became a hobby of mine and I was doing them regularly, fascinated by the puzzle each problem posed. The satisfaction derived when a complicated integral returns an elegant answer is hard to match.

Something I noticed when I began to pursue higher maths is the connection between seemingly unrelated topics. Euler's identity is perhaps the best example of this, where the constants e, π and i come together in perfect harmony. The Weierstrass substitution, through which the trigonometric functions can be expressed as rational functions of a variable t, is also compelling. This connectedness has a certain kind of beauty to it, not to mention the powerful implication that everything in maths is linked in some way we cannot grasp yet.

As a result of my journey into calculus, I was able to participate in the Senior Physics Challenge 2019, where I completed over 600 challenging questions in an eight-month period. This led to me being one of 41 students invited to a four-day residential at Cambridge University at the start of July. At the famous Cavendish Laboratory, Professor Mark Warner delivered a series of enthralling lectures in which he gave us a rigorous mathematical introduction to quantum mechanics. I was finally able to make sense of ideas I had run into previously like eigenvalues, eigenstates, the Schrödinger wave equation, infinite and finite potential wells, and forbidden regions. I also learnt about how the structure of atoms, and thus of the universe, is governed by the complex interplay of electrical attraction and kinetic energy of localisation.

The residential prompted me to write this paper, returning to where it all began in Year 9 (when I got my first look at quantum physics) but with a more informed perspective and an in-depth calculus-based approach which lent clarity to this inherently unintuitive field. I truly relished writing this paper and hope you can draw some inspiration from it!

My advice to any students who want to get into research is simple: don't get overwhelmed. The amount of maths out there is mind-boggling, and it is easy to get put off or disillusioned, and wonder how you are ever going to understand it all. I must confess this a feeling I have dealt with a multitude of times, not only while researching material for this paper, but since the beginning of my journey last summer. It's almost as if the more you advance, the more acutely aware you become of how little you know.

When these disheartening thoughts occur, it is important to appreciate that learning is a continuous and gradual process. There's no escaping the fact that you need to know the fundamentals to progress onto more difficult subject matter. Even the brightest minds had to start somewhere; there's no need to be daunted. So keep at it and you'll end up surprising yourself. I wish you all the best on you mathematical adventures!

2 Introduction

A differential equation is an equation relating a function and its derivatives. Solutions to these equations are not numerical values, but instead, are functions/curves.

In this paper, we will be using power series to find solutions to a particular class of differential equations: homogeneous, second-order ordinary differential equations with variable coefficients.

First, let us understand some of this terminology:

- An **ordinary** differential equation (ODE) involves functions of **only one** independent variable and their derivatives.
- The **order** of a differential equation indicates the **highest** derivative present. So, a second-order equation contains **up to** second derivatives.
- A **homogeneous** differential equation of the second-order is of the form:

  $$a_0(x)y + a_1(x)\frac{dy}{dx} + a_2(x)\frac{d^2y}{dx^2} = 0$$

  All the items are proportional to a derivative of y or y itself, and hence, the sum of the items is equal to zero.
- A differential equation is said to have **variable coefficients** if the function y and its derivatives are multiplied by other functions (of the same independent variable).

  In other words, looking at the form above, $a_0(x)$, $a_1(x)$ and $a_2(x)$ are **not** constants.

Next, let us briefly recap **power series**.

A power series (in a single variable x) is an infinite series that takes the form:

$$\boxed{\sum_{n=0}^{\infty} a_n(x-c)^n = a_0 + a_1(x-c) + a_2(x-c)^2 + \dots}$$

where a_n is the coefficient of the nth term and c is a constant denoting the centre of the series.

An example of a power series is the Taylor series of a function about a point c (which can be real or complex):

$$\sum_{n=0}^{\infty} \frac{f^{(n)}(c)}{n!}(x-c)^n = f(c) + \frac{f'(c)}{1!}(x-c) + \frac{f''(c)}{2!}(x-c)^2 + \frac{f'''(c)}{3!}(x-c)^3 + \cdots$$

Note that the function must be infinitely differentiable.

In many situations, the centre of a power series is equal to zero; indeed, when using power series to solve ODEs, we tend to find solutions about $x = 0$.

We would write such a power series as:

$$\sum_{n=0}^{\infty} a_n x^n = a_0 + a_1 x + a_2 x^2 + \dots$$

A Maclaurin series is a special case of the Taylor series centred at 0:

$$\sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} x^n = f(0) + \frac{f'(0)}{1!}x + \frac{f''(0)}{2!}x^2 + \frac{f'''(0)}{3!}x^3 + \cdots$$

When applying power series to ODEs, being able to spot common power series and identify the functions they represent may be useful. Below are a few basic Maclaurin expansions represented as power series:

$$\begin{aligned}
\sin(x) &= x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n\, x^{2n+1}}{(2n+1)!} \\
\cos(x) &= 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots = \sum_{n=0}^{\infty} \frac{(-1)^n\, x^{2n}}{(2n)!} \\
e^x &= 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots = \sum_{n=0}^{\infty} \frac{x^n}{n!} \\
\sinh(x) &= x + \frac{x^3}{3!} + \frac{x^5}{5!} + \frac{x^7}{7!} + \cdots = \sum_{n=0}^{\infty} \frac{x^{2n+1}}{(2n+1)!} \\
\cosh(x) &= 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \frac{x^6}{6!} + \cdots = \sum_{n=0}^{\infty} \frac{x^{2n}}{(2n)!}
\end{aligned}$$

Another prerequisite to solving ODEs is **combining** power series. All series must have the **same power on the x term** and the **same starting index** before they can be combined.

Consider this problem:

$$\sum_{n=1}^{\infty} n a_n x^{n-1} + \sum_{n=0}^{\infty} a_n x^{n+2}$$

For each power series, we let k equal to the power on the x term.

$$k = n - 1 \qquad\qquad k = n + 2$$

$$n = k + 1 \qquad\qquad n = k - 2$$

Using that substitution, we can transform the power series as follows:

$$\sum_{k=0}^{\infty} (k+1) a_{k+1} x^k + \sum_{k=2}^{\infty} a_{k-2} x^k$$

Now we have the same power on the x terms, but the indices of the power series do not match. In a situation like this, we move all indices to match the highest one. To make the first power series have an index of two, we can write its first two terms separately:

$$a_1 + 2a_2\, x + \sum_{k=2}^{\infty} (k+1) a_{k+1}\, x^k + \sum_{k=2}^{\infty} a_{k-2}\, x^k$$

Since the two conditions have been met, we can write the above expression as:

$$a_1 + 2a_2\, x + \sum_{k=2}^{\infty} x^k \left[(k+1) a_{k+1} + a_{k-2}\right]$$

A fact crucial to using power series in differential equations is that if we have a power series that equals zero, **all of the coefficients within the power series must also be zero.** For example, given the following:

$$\sum_{k=2}^{\infty} x^k \big[(k+1)a_{k+1} + a_{k-2}\big] = 0$$

...we may conclude that:

$$(k+1)a_{k+1} + a_{k-2} = 0$$

The last thing to know about power series is how to differentiate them.

$$f(x) = \sum_{n=0}^{\infty} a_n \, x^n$$

Applying the power rule:

$$f'(x) = \sum_{n=0}^{\infty} n \, a_n \, x^{n-1}$$

Since the first term (when $n = 0$) is 0, we can also write the above result with an index of 1:

$$f'(x) = \sum_{n=1}^{\infty} n \, a_n \, x^{n-1}$$

Applying the same logic, the second derivative is:

$$f''(x) = \sum_{n=0}^{\infty} n(n-1) \, a_n \, x^{n-2} = \sum_{n=2}^{\infty} n(n-1) \, a_n \, x^{n-2}$$

3 The power series method to solve ODEs

Now that we have all the required skills, we can begin to actually solve differential equations with power series.

The main idea with this method is to assume a power series form for the solution (centre $x = 0$), rewrite the differential equation in terms of power series, combine the series, and obtain a recurrence relation.

Let us illustrate this with an example:

$$(x^2 + 1)y'' - 4xy' + 6y = 0$$

Substituting our series expressions for y and its derivatives yields:

$$(x^2 + 1) \sum_{n=2}^{\infty} n(n-1) \, a_n \, x^{n-2} - 4x \sum_{n=1}^{\infty} n \, a_n \, x^{n-1} + 6 \sum_{n=0}^{\infty} a_n \, x^n = 0$$

Distributing:

$$\sum_{n=2}^{\infty} n(n-1) \, a_n \, x^{n-2} + \sum_{n=2}^{\infty} n(n-1) \, a_n \, x^n - \sum_{n=1}^{\infty} 4n \, a_n \, x^n + \sum_{n=0}^{\infty} 6a_n \, x^n = 0$$

Shifting the indices of the power series:

$$\sum_{k=0}^{\infty}(k+2)(k+1)\,a_{k+2}\,x^k+\sum_{k=2}^{\infty}k(k-1)\,a_k\,x^k-\sum_{k=1}^{\infty}4k\,a_k\,x^k+\sum_{k=0}^{\infty}6a_k\,x^k=0$$

We can write the second power series with a starting index of 0, since the first and second terms would both be zero. Similarly, the third series could begin with an index of 0 since that extra term would be 0.

$$\sum_{k=0}^{\infty}(k+2)(k+1)\,a_{k+2}\,x^k+\sum_{k=0}^{\infty}k(k-1)\,a_k\,x^k-\sum_{k=0}^{\infty}4k\,a_k\,x^k+\sum_{k=0}^{\infty}6a_k\,x^k=0$$

Now that all the series have the same index, we are ready to combine them.

$$\sum_{k=0}^{\infty}x^k\big[(k+2)(k+1)a_{k+2}+k(k-1)a_k-4ka_k+6a_k\big]=0$$

$$(k+2)(k+1)a_{k+2}+k(k-1)a_k-4ka_k+6a_k=0$$

To get our recurrence relation:

$$(k+2)(k+1)a_{k+2}+a^k[k(k-1)-4k+6]=0$$

$$(k+2)(k+1)a_{k+2}=-a^k[k^2-5k+6]$$

$$a_{k+2}=-\frac{(k-3)(k-2)}{(k+2)(k+1)}a^k$$

Here, we can see that the kth coefficient is determined by the $(k-2)$th coefficient. When this is the case, we can formulate our solution in terms of odd and even functions separately.

Trying values for k:

When $k=0$, $a_2=-3a_0$

When $k=1$, $a_3=-\frac{1}{3}a_1$

When $k=2$, $a_4=0$

When $k=3$, $a_5=0$

From a_4 onwards, all the coefficients are 0. Thus, both series - even (multiples of a_0) and odd (multiples of a_1) - terminate. This is quite unusual - usually only one of them will terminate.

The solution is of the form:

$$y=a_0+a_1x+a_2x^2+a_3x^3+a_4x^4\cdots$$

With our knowledge of the coefficients, we can conclude:

$$y(x)=a_0(1-3x^2)+a_1\left(x-\frac{1}{3}x^3\right)$$

4 Particles confined to a triangular potential well

4.1 What is a triangular well and why is it important?

A triangular well is formed of a linear potential $V(x)$ - $\frac{dV}{dx}$ is constant - which is bound by an infinite barrier at $x = 0$.

The potential is created by a constant electric field ε.

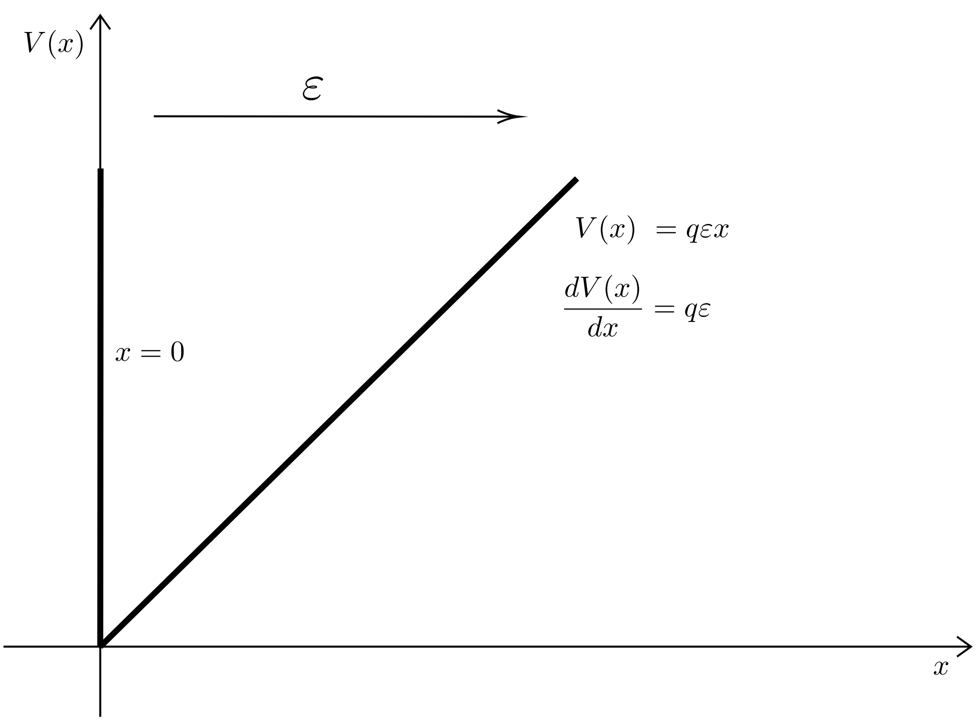
Since $\varepsilon = \frac{F}{q}$, where F is force and q is charge, we can rearrange this to say:

$$F = q\varepsilon$$

We also know that $E = Fd$ (or $W = Fd$) . If we apply this to our situation, we can say that $V = Fx$, where V is electrical energy or work done by the electric field and x is distance. Using our previously derived expression for F:

$$\therefore V(x) = q\varepsilon x$$

Representing this potential well on a graph makes its triangular nature clear:



These wells play a significant role in semi-conductor and transistor design. A noteworthy example is the high-electron-mobility transistor (HEMT) which confines electrons to the triangular well produced when different semi-conducting materials are juxtaposed to create a heterojunction.

These electrons have very high mobility (a measure of how fast they can move through a semi-conductor under the influence of an electric field), much greater than the MOSFETs (metal-oxide-semiconductor field-effect transistors) which are conventionally used.

HEMTs are used in a lot of high-frequency electronics such as radar equipment, satellite receivers and mobile phones.

4.2 Airy differential equation

The Airy differential equation is vital to solving the problem of the triangular well:

$$\boxed{y'' - xy = 0}$$

Assuming a power series form for the solution and substituting in our series expressions for y and its derivatives yields:

$$\sum_{n=2}^{\infty} n(n-1)\, a_n\, x^{n-2} - x \sum_{n=0}^{\infty} a_n\, x^n = 0 \Longrightarrow \sum_{n=2}^{\infty} n(n-1)\, a_n\, x^{n-2} - \sum_{n=0}^{\infty} a_n\, x^{n+1} = 0$$

Shifting the indices of the power series and combining them:

$$\sum_{k=0}^{\infty}(k+2)(k+1)\, a_{k+2}\, x^k - \sum_{k=1}^{\infty} a_{k-1}\, x^k = 0$$

$$2a_2 + \sum_{k=1}^{\infty}(k+2)(k+1)\, a_{k+2}\, x^k - \sum_{k=1}^{\infty} a_{k-1}\, x^k = 0$$

$$\therefore 2a_2 + \sum_{k=1}^{\infty} x^k[(k+2)(k+1)\, a_{k+2} - a_{k-1}\,] = 0$$

All the terms on the left-hand side of the equation must also equal to zero. Therefore:

$$2a_2 = 0; \;\; a_2 = 0$$

$$\sum_{k=1}^{\infty} x^k[(k+2)(k+1)\, a_{k+2} - a_{k-1}\,] = 0 \Rightarrow (k+2)(k+1)\, a_{k+2} - a_{k-1} \; = 0$$

We can now get a recurrence relation:

$$(k+2)(k+1)\, a_{k+2} = a_{k-1}$$

$$a_{k+2} = \frac{a_{k-1}}{(k+2)(k+1)}$$

Now we try values of k:

When $k = 0$, $a_2 = 0$ (previously determined)

When $k = 1$, $a_3 = \dfrac{a_0}{6}$

When $k = 2$, $a_4 = \dfrac{a_1}{12}$

When $k = 3$, $a_5 = \dfrac{a_2}{20} = 0$

When $k = 4$, $a_6 = \dfrac{a_3}{30} = \dfrac{a_0}{180}$

When $k = 5$, $a_7 = \dfrac{a_4}{42} = \dfrac{a_1}{504}$

When $k = 6$, $a_8 = \dfrac{a_5}{56} = 0$

The solution is of the form:

$$y(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4 \cdots$$

With our knowledge of the coefficients, we can conclude:

$$\begin{aligned} y(x) &= a_0 + a_1x + 0x^2 + \frac{a_0}{6}x^3 + \frac{a_1}{12}x^4 + 0x^5 + \frac{a_0}{180}x^6 + \frac{a_1}{504}x^7 + 0x^8 + \cdots \\ &= a_0 \underbrace{\left(1 + \frac{x^3}{6} + \frac{x^6}{180} + \cdots\right)}_{f(x)} + a_1 \underbrace{\left(x + \frac{x^4}{12} + \frac{x^7}{504} + \cdots\right)}_{g(x)} \end{aligned}$$

The series $f(x)$ and $g(x)$ are used to construct the Airy functions $\text{Ai}(x)$ and $\text{Bi}(x)$, which are linearly independent solutions to the Airy differential equation, i.e. $y = c_1\text{Ai}(x) + c_2\text{Bi}(x)$

The **Airy function of the first kind** $\text{Ai}(x)$ is written as:

$$\begin{aligned} \text{Ai}(x) &= \text{Ai}(0)\, f(x) + \text{Ai}'(0)\, g(x) \\ &= \text{Ai}(0) \left(1 + \frac{x^3}{6} + \frac{x^6}{180} + \cdots\right) + \text{Ai}'(0) \left(x + \frac{x^4}{12} + \frac{x^7}{504} + \cdots\right) \end{aligned}$$

where $\text{Ai}(0) = \dfrac{1}{3^{2/3}\Gamma(\frac{2}{3})}$ and $\text{Ai}'(0) = -\dfrac{1}{3^{1/3}\Gamma(\frac{1}{3})}$

Therefore:

$$\boxed{\text{Ai}(x) = \frac{1}{3^{2/3}\Gamma(\frac{2}{3})} \left(1 + \frac{x^3}{6} + \frac{x^6}{180} + \cdots\right) - \frac{1}{3^{1/3}\Gamma(\frac{1}{3})} \left(x + \frac{x^4}{12} + \frac{x^7}{504} + \cdots\right)}$$

The gamma function is defined as:

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

Thus, via numerical integration:

$$\Gamma\left(\frac{2}{3}\right) = \int_0^\infty t^{-\frac{1}{3}}e^{-t}dt \approx 1.354 \Rightarrow \text{Ai}(0) \approx 0.355$$

$$\Gamma\left(\frac{1}{3}\right) = \int_0^\infty t^{-\frac{2}{3}}e^{-t}dt \approx 2.679 \Rightarrow \text{Ai}'(0) \approx -0.259$$

Using these values, we can say:

$$\boxed{\text{Ai}(x) \approx 0.355 \left(1 + \frac{x^3}{6} + \frac{x^6}{180} + \cdots\right) - 0.259 \left(x + \frac{x^4}{12} + \frac{x^7}{504} + \cdots\right)}$$

The **Airy function of the second kind** $\text{Bi}(x)$ is written as:

$$\begin{aligned} \text{Bi}(x) &= \text{Bi}(0)\, f(x) + \text{Bi}'(0)\, g(x) \\ &= \text{Bi}(0) \left(1 + \frac{x^3}{6} + \frac{x^6}{180} + \cdots\right) + \text{Bi}'(0) \left(x + \frac{x^4}{12} + \frac{x^7}{504} + \cdots\right) \end{aligned}$$

where $\text{Bi}(0) = \dfrac{1}{3^{1/6}\Gamma(\frac{2}{3})}$ and $\text{Bi}'(0) = \dfrac{3^{1/6}}{\Gamma(\frac{1}{3})}$

Consequently:

$$\boxed{\mathrm{Bi}(x) = \frac{1}{3^{1/6}\Gamma(\frac{2}{3})}\left(1 + \frac{x^3}{6} + \frac{x^6}{180} + \cdots\right) + \frac{3^{1/6}}{\Gamma(\frac{1}{3})}\left(x + \frac{x^4}{12} + \frac{x^7}{504} + \cdots\right)}$$

Since we know $\Gamma\left(\dfrac{2}{3}\right)$ to be approximately equal to 1.354 and $\Gamma\left(\dfrac{1}{3}\right)$ to be approximately 2.679, we can compute the following:

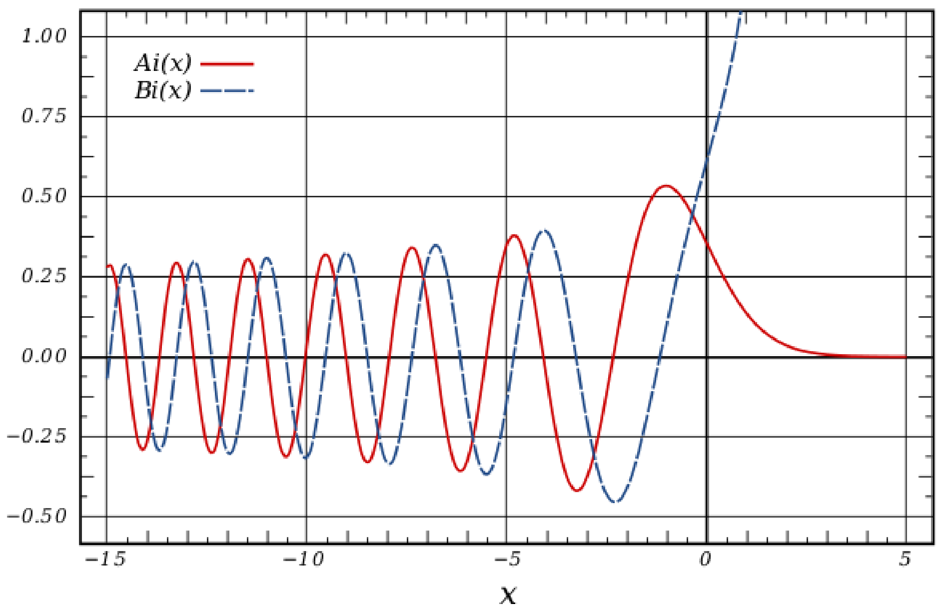
$$\mathrm{Bi}(0) \approx 0.615$$

$$\mathrm{Bi}'(0) \approx 0.448$$

Hence:

$$\boxed{\mathrm{Bi}(x) \approx 0.615\left(1 + \frac{x^3}{6} + \frac{x^6}{180} + \cdots\right) + 0.448\left(x + \frac{x^4}{12} + \frac{x^7}{504} + \cdots\right)}$$

If we plot the two Airy functions on a graph, we get:



4.3 Solving the Schrödinger equation for the triangular potential well

The Schrödinger equation in this case can be rearranged to the Airy equation, which is why the Airy functions are critical.

The time-independent Schrödinger equation (in one dimension) is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\,\psi(x) = E\,\psi(x)$$

If we replace $V(x)$ with $q\varepsilon x$, the Schrödinger equation becomes:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + q\varepsilon x\,\psi_n(x) = E_n\,\psi_n(x)$$

where E_n represents the nth stationary state/eigenstate of the system.

We can manipulate this as follows:

$$
\begin{aligned}
\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} &= q\varepsilon x\,\psi_n(x) - E_n\,\psi_n(x) \\
&= \psi_n(x)(q\varepsilon x - E_n) \\
\frac{\hbar^2}{2m}\frac{1}{q\varepsilon}\frac{d^2\psi_n(x)}{dx^2} &= \frac{1}{q\varepsilon}\psi_n(x)(q\varepsilon x - E_n) \\
&= \psi_n(x)\left(x - \frac{E_n}{q\varepsilon}\right) \\
\frac{d^2\psi_n(x)}{dx^2} &= \frac{2mq\varepsilon}{\hbar^2}\psi_n(x)\left(x - \frac{E_n}{q\varepsilon}\right)
\end{aligned}
$$

Let $z = \beta\left(x - \frac{E_n}{q\varepsilon}\right)$, where β is a normalisation factor (to ensure that the equation ends up matching the Airy equation).

Differentiating both sides with respect to x:

$$\frac{dz}{dx} = \beta$$

$$dz = \beta\,dx \Rightarrow dx = \frac{dz}{\beta}$$

Substituting all this back into our rearranged equation and expressing everything in terms of z:

$$
\begin{aligned}
\frac{d^2\psi_n(z)}{\left(\frac{dz}{\beta}\right)^2} &= \frac{2mq\varepsilon}{\hbar^2}\psi_n(z)\,z\beta^{-1} \\
\beta^2\frac{d^2\psi_n(z)}{dz^2} &= \frac{2mq\varepsilon}{\hbar^2}\,\psi_n(z)\,z\beta^{-1} \\
\frac{d^2\psi_n(z)}{dz^2} &= \frac{2mq\varepsilon}{\hbar^2}\,\psi_n(z)\,z\,\beta^{-3}
\end{aligned}
$$

For this equation to become the Airy equation, the quantity $\left(\frac{2mq\varepsilon}{\hbar^2}\,\beta^{-3}\right)$ must equal to 1.

Therefore:

$$\frac{2mq\varepsilon}{\hbar^2} = \beta^3 \Rightarrow \beta = \sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}$$

Now that we have a value for the normalisation factor, we can conclude that:

$$z = \sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\left(x - \frac{E_n}{q\varepsilon}\right)$$

Solving the equation $\frac{d^2\psi_n(z)}{dz^2} = \psi_n(z)\,z$, we obtain the Airy functions as two solutions:

$$\psi_n(z) = A\,\mathrm{Ai}(z) + B\,\mathrm{Bi}(z)$$

where A and B are constants ensuring that the wavefunctions are normalised i.e.

$$\int_0^\infty |\psi_n(z)|^2 dz = 1$$

However, looking back to the graph of the Airy functions, we see that the Airy function of the second kind $\mathrm{Bi}(z)$ diverges (goes to infinity) for positive values of z. Since it does not go to zero as $z \to \infty$, it is not possible to normalise the wavefunction and we can reject $\mathrm{Bi}(z)$ as a solution. This leaves only $\mathrm{Ai}(z)$ (which decays exponentially when $z > 0$).

$$\therefore \psi_n(z) = A\,\mathrm{Ai}(z)$$

Converting so that we express the wavefunction in terms of x:

$$\boxed{\psi_n(x) = A\,\mathrm{Ai}\left[\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\left(x - \frac{E_n}{q\varepsilon}\right)\right]}$$

We can also derive an **equation for the energy eigenvalues** E_n.

Since there is an infinite barrier at $x = 0$:

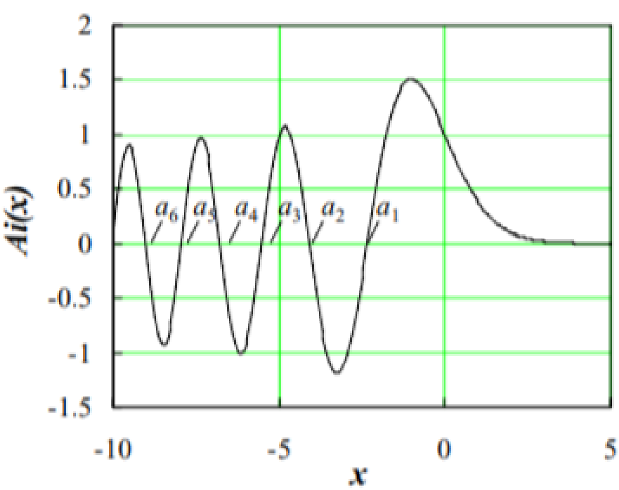
$$\psi_n(0) = 0$$

$$\therefore A\,\mathrm{Ai}\left[-\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\frac{E_n}{q\varepsilon}\right] = 0$$

The normalisation constant A cannot be 0. For that reason:

$$\mathrm{Ai}\left[-\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\frac{E_n}{q\varepsilon}\right] = 0$$

Let α_n denote the x co-ordinate of the nth zero of $\mathrm{Ai}(x)$ (the zeroes of the function are shown below).



Hence,

$$\alpha_n = -\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\frac{E_n}{q\varepsilon}$$

As a result:

$$E_n = -\alpha_n\, q\,\varepsilon\sqrt[3]{\frac{\hbar^2}{2mq\varepsilon}}$$

Taking the $q\varepsilon$ into the cube root:

$$\boxed{E_n = -\alpha_n\sqrt[3]{\frac{\hbar^2 q^2 \varepsilon^2}{2m}}}$$

Lastly, we can **compute the normalisation constant** A. For the wavefunction to be normalised:

$$\int_0^\infty |\psi_n(x)|^2 dx = 1$$

We integrate from 0 to ∞ since there is an infinite barrier at $x = 0$ (we cannot go beyond that point into negative x values).

$$\therefore \int_0^\infty A^2 \, \mathrm{Ai}^2 \left[\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}} \left(x - \frac{E_n}{q\varepsilon} \right) \right] dx = 1$$

We can take the constant out as follows:

$$\int_0^\infty \mathrm{Ai}^2 \left[\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}} \left(x - \frac{E_n}{q\varepsilon} \right) \right] dx = \frac{1}{A^2}$$

Let us define a new function $f(x)$:

$$f(x) = \sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}} \left(x - \frac{E_n}{q\varepsilon} \right)$$

Hence:

$$\frac{df(x)}{dx} = \sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}} \Rightarrow df(x) = \sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}} dx$$

Using this and changing the bounds of the integral:

$$\sqrt[3]{\frac{\hbar^2}{2mq\varepsilon}} \int_{f(0)}^{f(\infty)} \mathrm{Ai}^2 \left[f(x) \right] df(x) = \frac{1}{A^2}$$

Note that as $x \to \infty$, $f(x) \to \infty$. So, we can write the earlier equation as:

$$\int_{f(0)}^\infty \mathrm{Ai}^2 \left[f(x) \right] df(x) = \frac{1}{A^2} \sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}$$

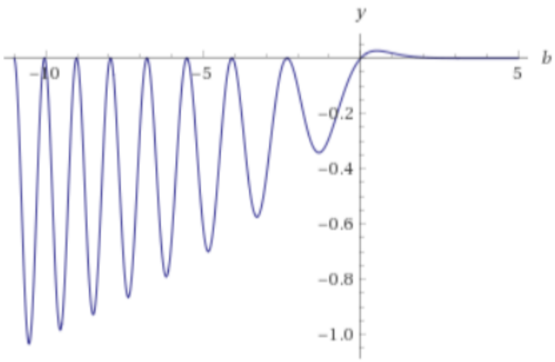
An important identity we will need here is:

$$\boxed{\int \mathrm{Ai}^2(x) dx = x \mathrm{Ai}^2(x) - \mathrm{Ai}'^2(x) + c}$$

Returning to the improper integral we had arrived at:

$$\begin{aligned}
\int_{f(0)}^\infty \mathrm{Ai}^2 \left[f(x) \right] df(x) &= \lim_{b \to \infty} \int_{f(0)}^b \mathrm{Ai}^2 \left[f(x) \right] df(x) \\
&= \lim_{b \to \infty} \left[f(x) \, \mathrm{Ai}^2[f(x)] - \mathrm{Ai}'^2[f(x)] \Big|_{f(0)}^b \right] \\
&= \lim_{b \to \infty} \left[b \, \mathrm{Ai}^2(b) - \mathrm{Ai}'^2(b) - \Big(f(0) \, \mathrm{Ai}^2 \left[f(0) \right] - \mathrm{Ai}'^2[f(0)] \Big) \right] \\
&= \lim_{b \to \infty} \left[b \, \mathrm{Ai}^2(b) - \mathrm{Ai}'^2(b) + \mathrm{Ai}'^2[f(0)] - f(0) \, \mathrm{Ai}^2 \left[f(0) \right] \right] \\
&= \lim_{b \to \infty} b \, \mathrm{Ai}^2(b) - \lim_{b \to \infty} \mathrm{Ai}'^2(b) + \mathrm{Ai}'^2[f(0)] - f(0) \, \mathrm{Ai}^2 \left[f(0) \right] \\
&= \lim_{b \to \infty} b \, \mathrm{Ai}^2(b) - 0 + \mathrm{Ai}'^2[f(0)] - f(0) \, \mathrm{Ai}^2 \left[f(0) \right]
\end{aligned}$$

To evaluate the remaining limit, we can graph the function $b\text{Ai}^2(b)$:



Observing the behaviour as $b \to \infty$, we see that the function goes to 0. With this:

$$\begin{aligned}\int_{f(0)}^{\infty} \text{Ai}^2\left[f(x)\right] df(x) &= 0 - 0 + \text{Ai}'^{\,2}[f(0)] - f(0)\,\text{Ai}^2\left[f(0)\right] \\ &= \text{Ai}'^{\,2}[f(0)] - f(0)\,\text{Ai}^2\left[f(0)\right]\end{aligned}$$

Now we can conclude that:

$$\text{Ai}'^{\,2}[f(0)] - f(0)\,\text{Ai}^2\left[f(0)\right] = \frac{1}{A^2}\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}$$

$$\therefore A = \left(\frac{\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}}{\text{Ai}'^{\,2}[f(0)] - f(0)\,\text{Ai}^2\left[f(0)\right]}\right)^{1/2}$$

Since $f(0) = -\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\frac{E_n}{q\varepsilon}$, $A = \left(\frac{\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}}{\text{Ai}'^{\,2}\left(-\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\frac{E_n}{q\varepsilon}\right) + \sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\frac{E_n}{q\varepsilon}\,\text{Ai}^2\left(-\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\frac{E_n}{q\varepsilon}\right)}\right)^{1/2}$

When we considered the infinite barrier at $x = 0$ previously, we deduced that:

$$\text{Ai}\left[-\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\frac{E_n}{q\varepsilon}\right] = 0$$

This means that A reduces to:

$$A = \left(\frac{\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}}{\text{Ai}'^{\,2}\left[-\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\frac{E_n}{q\varepsilon}\right]}\right)^{1/2}$$

And hence:

$$\boxed{\psi_n(x) = \left(\frac{\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}}{\text{Ai}'^{\,2}\left[-\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\frac{E_n}{q\varepsilon}\right]}\right)^{1/2} \text{Ai}\left[\sqrt[3]{\frac{2mq\varepsilon}{\hbar^2}}\left(x - \frac{E_n}{q\varepsilon}\right)\right]}$$

5 The quantum harmonic oscillator

5.1 What is the quantum oscillator and why is it important?

In classical mechanics, a harmonic oscillator describes any physical system which, when displaced from equilibrium by x, comes up against a restoring force F (acting towards equilibrium) directly proportional to x. An example of such a system is a mass on a spring or a simple pendulum:

This relationship between F and x is given by Hooke's Law:

$$F = -kx$$

where k is the constant of proportionality (called the spring constant) and the negative sign indicates that the force and displacement are in opposite directions.

From this, we can calculate the work done by the harmonic oscillator using an integral ($W = Fx$ applies only for a constant force):

$$\begin{aligned} W &= \int_0^x F\,dx \\ &= -k\int_0^x x\,dx \\ &= -\frac{1}{2}kx^2 \end{aligned}$$

Negative work corresponds to an increase in the particle's potential energy. Thus:

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

Note that this harmonic potential must therefore increase quadratically either side of $x = 0$.

The equation of motion for the harmonic oscillator(by combining Newton's second law and Hooke's law):

$$m\frac{d^2\,x}{dt^2} = -kx$$

$$\therefore \frac{d^2\,x}{dt^2} = -\frac{k}{m}x \equiv -\omega^2 x$$

where $\omega = \sqrt{\frac{k}{m}}$ is angular frequency.

When we begin to look at very small energies, the laws of classical mechanics no longer apply to the oscillator; instead, quantum mechanics takes over and we are dealing with a quantum oscillator.

A simple example of such an oscillator is a vibrating diatomic molecule. From this starting point, we can understand more complicated vibrations in large compounds, and discover how atoms vibrate in a lattice structure.

5.2 Hermite differential equation

The Hermite equation is an integral part of solving the Schrödinger equation for the quantum oscillator, so it is imperative that we are able to solve it:

$$\boxed{y'' - 2xy' + 2\lambda y = 0}$$

Presuming that the solution takes the form of a power series

$$\sum_{n=0}^{\infty} n(n-1)a_n\, x^{n-2} - 2x\sum_{n=0}^{\infty} na_n\, x^{n-1} + 2\lambda\sum_{n=0}^{\infty} a_n\, x^n = 0$$
$$\sum_{n=2}^{\infty} n(n-1)a_n\, x^{n-2} - \sum_{n=1}^{\infty} 2na_n\, x^n + \sum_{n=0}^{\infty} 2\lambda a_n\, x^n = 0$$

If we make the substitution that $k = n-2$ for the first power series, and $k = n$ for the other two:

$$\sum_{k=0}^{\infty}(k+2)(k+1)a_{k+2}\, x^k - \sum_{k=1}^{\infty} 2ka_k\, x^k + \sum_{k=0}^{\infty} 2\lambda a_k\, x^k = 0$$

To make the starting indices of the power series equal, we can say:

$$2a_2 + \sum_{k=1}^{\infty}(k+2)(k+1)a_{k+2}\, x^k - \sum_{k=1}^{\infty} 2ka_k\, x^k + 2\lambda a_0 + \sum_{k=1}^{\infty} 2\lambda a_k\, x^k = 0$$

Combining the power series:

$$2a_2 + 2\lambda a_0 + \sum_{k=1}^{\infty}(k+2)(k+1)a_{k+2}\, x^k - 2ka_k\, x^k + 2\lambda a_k\, x^k = 0$$
$$2a_2 + 2\lambda a_0 + \sum_{k=1}^{\infty} x^k[(k+2)(k+1)a_{k+2} - 2ka_k + 2\lambda a_k] = 0$$

From this, we can glean the following:

$$2a_2 + 2\lambda a_0 = 0 \Rightarrow a_2 = -\lambda a_0$$

We can also get the recurrence relation from the above result:

$$(k+2)(k+1)a_{k+2} - 2ka_k + 2\lambda a_k = 0$$
$$(k+2)(k+1)a_{k+2} - a_k(2k - 2\lambda) = 0$$
$$a_{k+2} = \frac{2(k-\lambda)a_k}{(k+2)(k+1)}$$

Since the kth coefficient is determined by the $(k-2)$th coefficient, we will be able to write the solution in two parts: one odd (odd powers of x) and one even (even powers of x).

If we try different values of k:

When $k = 0$, $a_2 = \dfrac{-2\lambda}{2}a_0 = -\lambda a_0$

When $k = 1$, $a_3 = \dfrac{2(1-\lambda)}{6}a_1 = \dfrac{(1-\lambda)}{3}a_1$

When $k = 2$, $a_4 = \dfrac{2(2-\lambda)}{12}a_2 = \dfrac{(2-\lambda)}{6}a_2 = \dfrac{\lambda(\lambda-2)}{6}a_0$

When $k = 3$, $a_5 = \dfrac{2(3-\lambda)}{20}a_3 = \dfrac{(3-\lambda)}{10}a_3 = \dfrac{(1-\lambda)(3-\lambda)}{30}a_1$

When $k = 4$, $a_6 = \dfrac{2(4-\lambda)}{30}a_4 = \dfrac{(4-\lambda)}{15}a_4 = \dfrac{\lambda(4-\lambda)(\lambda-2)}{90}a_0$

Since y is a power series, the solution is of the form:

$$y(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4 \cdots$$

If we put the coefficients we have calculated into this, we get two linearly independent solutions (one odd, one even):

$$\begin{aligned} y(x) &= a_0 + a_1x - \lambda a_0x^2 + \frac{(1-\lambda)}{3}a_1x^3 + \frac{\lambda(\lambda-2)}{6}a_0x^4 + \frac{(1-\lambda)(3-\lambda)}{30}a_1x^5 + \frac{\lambda(4-\lambda)(\lambda-2)}{90}a_0x^6 \cdots \\ &= a_0\left(1 - \lambda x^2 + \frac{\lambda(\lambda-2)}{6}x^4 + \frac{\lambda(4-\lambda)(\lambda-2)}{90}x^6 \cdots\right) + a_1\left(x + \frac{(1-\lambda)}{3}x^3 + \frac{(1-\lambda)(3-\lambda)}{30}x^5 \cdots\right) \end{aligned}$$

We can now test different values for λ.

When $\lambda = 0$, $y = a_0 + a_1\left(x + \dfrac{1}{3}x^3 + \dfrac{1}{10}x^5 + \cdots\right)$

When $\lambda = 1$, $y = a_0\left(1 - x^2 - \dfrac{1}{6}x^4 - \dfrac{1}{30}x^6 - \cdots\right) + a_1x$

When $\lambda = 2$, $y = a_0(1-2x^2) + a_1\left(x - \dfrac{1}{3}x^3 - \dfrac{1}{30}x^5 - \cdots\right)$

When $\lambda = 3$, $y = a_0\left(1 - x^2 + \dfrac{1}{2}x^4 + \dfrac{1}{30}x^6 + \cdots\right) + a_1\left(x - \dfrac{2}{3}x^3\right)$

When $\lambda = 4$, $y = a_0\left(1 - 4x^2 + \dfrac{4}{3}x^4\right) + a_1\left(x - x^3 + \dfrac{1}{10}x^5 + \cdots\right)$

Note that for even values of λ, the even solution terminates whereas for odd values, the odd solution terminates.

The **Hermite polynomials** are the **normalised**, **bounded** (i.e. terminated) solutions to the Hermite differential equations.

The first few bounded polynomials are:

$\lambda = 0 \Rightarrow y = a_0$

$\lambda = 1 \Rightarrow y = a_1x$

$\lambda = 2 \Rightarrow y = a_0(1-2x^2) = a_0 - 2a_0x^2$

$\lambda = 3 \Rightarrow y = a_1\left(x - \dfrac{2}{3}x^3\right) = a_1x - \dfrac{2}{3}a_1x^3$

$\lambda = 4 \Rightarrow y = a_0\left(1 - 4x^2 + \dfrac{4}{3}x^4\right) = a_0 - 4a_0x^2 + \dfrac{4}{3}a_0x^4$

There are two ways of normalising these bounded polynomials. Physicists normalise them such that the leading coefficient of the polynomial (preceding the highest degree term x^n) is equal to 2^n. Using this, we can write the first few Hermite polynomials (according to physicists).

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$H_2(x) = 4x^2 + a_0$$

$$H_3(x) = 8x^3 + a_1 x$$

$$H_4(x) = 16x^4 - 4a_0 x^2 + a_0$$

We can plug these solutions into the differential equation to find the Hermite polynomials:

$$H_n(x)'' - 2xH_n(x)' + 2\lambda H_n(x) = 0$$

Doing this for the second Hermite polynomial:

$$\begin{aligned} 8 - 2x(8x) + 4(4x^2 + a_0) &= 0 \\ \therefore 4a_0 &= -8 \\ a_0 &= -2 \\ &\boxed{H_2 = 4x^2 - 2} \end{aligned}$$

With the third Hermite polynomial:

$$\begin{aligned} 48x - 2x(24x^2 + a_1) + 6(8x^3 + a_1 x) &= 0 \\ \therefore 4a_1 &= 48 \\ a_1 &= 12 \\ &\boxed{H_3 = 8x^3 + 12} \end{aligned}$$

For the fourth:

$$\begin{aligned} 192x^2 - 8a_0 - 2x(64x^3 - 8a_0 x) + 8(16x^4 - 4a_0 x^2 + a_0) &= 0 \\ \therefore 16a_0 &= 192 \\ a_0 &= 12 \\ &\boxed{H_4 = 16x^4 - 48x^2 + 12} \end{aligned}$$

Thus, the Hermite polynomials (physics) are:

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$H_2(x) = 4x^2 - 2$$

$$H_3(x) = 8x^3 + 12x$$

$$H_4(x) = 16x^4 - 48x^2 + 12$$

5.3 Solving the Schrödinger equation for the quantum harmonic oscillator

In this section, we will transform the Schrödinger equation we obtain into the Hermite equation, and see that the Hermite polynomials bring about the different eigenstates of the quantum oscillator.

The Schrödinger equation for the quantum harmonic oscillator, replacing $V(x)$ with $\frac{1}{2}kx^2$ is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + \frac{1}{2}kx^2\psi_n(x) = E_n\psi_n(x)$$

Rewriting the equation for angular frequency gives the following result:

$$k = m\omega^2$$

Hence,

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + \frac{1}{2}m\omega^2x^2\psi_n(x) &= E_n\psi_n(x) \\
\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} &= \frac{1}{2}m\omega^2x^2\psi_n(x) - E_n\psi_n(x) \\
\frac{d^2\psi_n(x)}{dx^2} &= \frac{2m}{\hbar^2}\left(\frac{1}{2}m\omega^2x^2 - E_n\right)\psi_n(x)
\end{aligned}$$

Brining all terms to the same side of the equation

$$\begin{aligned}
\frac{d^2\psi_n(x)}{dx^2} + \frac{2m}{\hbar^2}\left(E_n - \frac{1}{2}m\omega^2x^2\right)\psi_n(x) = 0 \\
\frac{d^2\psi_n(x)}{dx^2} + \left(\frac{2mE_n}{\hbar^2} - \frac{m^2\omega^2x^2}{\hbar^2}\right)\psi_n(x) = 0
\end{aligned}$$

Next, we non-dimensionalise the equation, to reduce the number of parameters (m, E_n, ω, etc.)

First, let us non-dimensionalise position. Consider the following term: $\dfrac{m^2\omega^2}{\hbar^2}$

Through dimensional analysis, we see that this term has the same dimensions as x^{-4}:

$$\begin{aligned}
\frac{m^2\omega^2}{\hbar^2} = \frac{m^2\frac{k}{m}}{\hbar^2} &= \frac{km}{\hbar^2} \\
k = \frac{F}{x} = \frac{ma}{x} &\Rightarrow \frac{[\text{kg}][\text{m}][\text{s}^{-2}]}{[\text{m}]} = [\text{kg}][\text{s}^{-2}] \\
\hbar &\Rightarrow [\text{kg}][\text{m}^2][\text{s}^{-1}] \\
\frac{km}{\hbar^2} &\Rightarrow \frac{[\text{kg}^2][\text{m}][\text{s}^{-2}]}{[\text{kg}^2][\text{m}^4][\text{s}^{-2}]} = [\text{m}^{-4}]
\end{aligned}$$

So, if we let $\sigma = \sqrt{\dfrac{\hbar}{m\omega}}$, it has the same dimensions as x.

Introducing another variable β such that

$$\beta = \frac{x}{\sigma} = \sqrt{\frac{m\omega}{\hbar}}x$$

makes it dimensionless.

Differentiating both sides with respect to x:

$$\frac{d\beta}{dx} = \sqrt{\frac{m\omega}{\hbar}} \Rightarrow d\beta = \sqrt{\frac{m\omega}{\hbar}}dx$$
$$\Rightarrow dx = \sqrt{\frac{\hbar}{m\omega}}d\beta$$

Using the above:

$$\frac{d^2\psi_n(x)}{dx^2} = \frac{m\omega}{\hbar}\frac{d^2\psi_n(\beta)}{d\beta^2}$$
$$\frac{m^2\omega^2x^2}{\hbar^2} = \frac{m^2\omega^2}{\hbar^2}\beta^2\frac{\hbar}{m\omega} = \frac{\beta^2 m\omega}{\hbar}$$

Substituting these values back into the rearranged Schrödinger equation:

$$\frac{m\omega}{\hbar}\frac{d^2\psi_n(\beta)}{d\beta^2} + \left(\frac{2mE_n}{\hbar^2} - \frac{\beta^2 m\omega}{\hbar}\right)\psi_n(\beta) = 0$$

Now, let us non-dimensionalise energy. The Planck-Einstein relation states that:

$$E = hf$$

Replacing frequency with angular frequency yields:

$$E = \hbar\omega$$

We could set $\varepsilon = \dfrac{E_n}{\hbar\omega}$ to create a dimensionless quantity and this would lead to:

$$\frac{m\omega}{\hbar}\frac{d^2\psi_n(\beta)}{d\beta^2} + \frac{m\omega}{\hbar}\left(2\varepsilon - \beta^2\right)\psi_n(\beta) = 0$$

$$\frac{d^2\psi_n(\beta)}{d\beta^2} + \left(2\varepsilon - \beta^2\right)\psi_n(\beta) = 0$$

To further simplify the final equation, we could instead set $\varepsilon = \dfrac{2E_n}{\hbar\omega}$. Doing this, we get:

$$\frac{d^2\psi_n(\beta)}{d\beta^2} + \left(\varepsilon - \beta^2\right)\psi_n(\beta) = 0$$

Applying asymptotic analysis and considering very large or very small values of β (i.e. $\beta \to \pm\infty$), the ε term becomes negligible:

$$\lim_{\beta\to\pm\infty}\frac{d^2\psi_n(\beta)}{d\beta^2} - \beta^2\psi_n(\beta) \approx 0$$
$$\lim_{\beta\to\pm\infty}\frac{d^2\psi_n(\beta)}{d\beta^2} \approx \beta^2\psi_n(\beta)$$

This gives us a trial solution matching the form of the Gaussian function:

$$\psi_n(\beta) = c_1 e^{\frac{\xi\beta^2}{2}}$$

where ξ is a constant.

Finding the second derivative

$$\frac{d^2 c_1 e^{\frac{\xi\beta^2}{2}}}{d\beta^2} = c_1\xi e^{\frac{\xi\beta^2}{2}} + c_1\xi^2\beta^2 e^{\frac{\xi\beta^2}{2}} = (\xi + \beta^2\xi^2)\psi_n(\beta)$$

If we apply the limit:

$$\begin{aligned} \lim_{\beta\to\pm\infty} \frac{d^2 c_1 e^{\frac{\xi\beta^2}{2}}}{d\beta^2} &= \lim_{\beta\to\pm\infty} (\xi + \beta^2\xi^2)\psi_n(\beta) \\ &\approx \beta^2\xi^2\psi_n(\beta) \\ \therefore \beta^2\xi^2\psi_n(\beta) &= \beta^2\psi_n(\beta) \\ \xi &= \pm 1 \end{aligned}$$

Consequently, we get two solutions:

$$\psi_n(\beta) = c_1 e^{\frac{\beta^2}{2}};\ \psi_n(\beta) = c_2 e^{\frac{-\beta^2}{2}}$$

Only the second solution is normalisable; integrating the square of the first solution between negative and positive infinity does not produce a finite result. We are left with:

$$\psi_n(\beta) = c_2 e^{\frac{-\beta^2}{2}}$$

On the basis of this and by generalising c_2 to a function of β, we assume a solution such that:

$$\psi_n(\beta) = f(\beta)\, e^{\frac{-\beta^2}{2}}$$

Differentiating twice:

$$\psi_n'(\beta) = f'(\beta)\, e^{\frac{-\beta^2}{2}} - f(\beta)\beta\, e^{\frac{-\beta^2}{2}}$$
$$\psi_n''(\beta) = f''(\beta) e^{\frac{-\beta^2}{2}} - 2\beta f'(\beta)\, e^{\frac{-\beta^2}{2}} + f(\beta)(\beta^2 - 1) e^{\frac{-\beta^2}{2}}$$

Plugging all these back into the non-dimensionalised differential equation and simplifying:

$$\begin{aligned} \frac{d^2\psi_n(\beta)}{d\beta^2} + \left(\varepsilon - \beta^2\right)\psi_n(\beta) &= 0 \\ f''(\beta) e^{\frac{-\beta^2}{2}} - 2\beta f'(\beta)\, e^{\frac{-\beta^2}{2}} + (\beta^2 - 1) f(\beta) e^{\frac{-\beta^2}{2}} + \left(\varepsilon - \beta^2\right) f(\beta)\, e^{\frac{-\beta^2}{2}} &= 0 \\ f''(\beta) e^{\frac{-\beta^2}{2}} - 2\beta f'(\beta)\, e^{\frac{-\beta^2}{2}} + (\varepsilon - 1) f(\beta) e^{\frac{-\beta^2}{2}} &= 0 \\ f''(\beta) - 2\beta f'(\beta) + (\varepsilon - 1) f(\beta) &= 0 \end{aligned}$$

This second-order differential equation we attain is the Hermite differential equation, provided that:

$$\varepsilon - 1 = 2\lambda \Rightarrow \varepsilon = 2\lambda + 1$$

If we replace the λ with an n, since they are both just constants and the convention we have been using is to denote the different eigenstates of the quantum harmonic oscillator using n:

$$\varepsilon = 2n + 1$$

Recalling that $\varepsilon = \dfrac{2E_n}{\hbar\omega}$:

$$\frac{2E_n}{\hbar\omega} = 2n + 1$$

$$E_n = \frac{\hbar\omega(2n+1)}{2}$$

$$\boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right);\ n = 0, 1, 2\cdots}$$

The energies are **quantised**! Observe the difference to classical mechanics, where the oscillator's energy can take on any positive value at all.

Another point to note is that while the classical oscillator has no energy (it is completely at rest) in its ground state, the quantum oscillator **does**:

$$E_0 = \frac{1}{2}\hbar\omega$$

This energy is called the **zero-point energy** and may imply that molecules (remembering a vibrating diatomic molecule is a simple quantum harmonic oscillator) are never fully still, even at 0K (absolute zero).

Going back to where we left off (having reached the Hermite equation), we see that the solutions for $f(\beta)$ are the Hermite polynomials $\mathrm{H}_\beta(x)$. To conclude:

$$\psi_n(\beta) = \mathrm{H}_n(\beta)e^{\frac{-\beta^2}{2}}$$

β is defined as:

$$\beta = \frac{x}{\sigma} = \sqrt{\frac{m\omega}{\hbar}}x$$

Hence, the wavefunction is:

$$\boxed{\psi_n(x) = a_n\,\mathrm{H}_n\left(\frac{x}{\sigma}\right)e^{\frac{-x^2}{2\sigma^2}}}$$

where a_n is the normalisation factor.

Fully expanded:

$$\boxed{\psi_n(x) = a_n\,\mathrm{H}_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{\frac{-m\omega x^2}{2\hbar}}}$$

Writing the first few eigenstates and eigenenergies for the quantum oscillator:

n	E_n	$\psi_n(x)$	
0	$E_0 = \dfrac{\hbar\omega}{2}$	$\psi_0(x) = a_0\,e^{\frac{-x^2}{2\sigma^2}}$	$= a_0\,e^{\frac{-m\omega x^2}{2\hbar}}$
1	$E_0 = \dfrac{3\hbar\omega}{2}$	$\psi_0(x) = a_1\,\dfrac{2x}{\sigma}\,e^{\frac{-x^2}{2\sigma^2}}$	$= a_1\left(2\sqrt{\dfrac{m\omega}{\hbar}}x\right)e^{\frac{-m\omega x^2}{2\hbar}}$
2	$E_0 = \dfrac{5\hbar\omega}{2}$	$\psi_0(x) = a_2\left(\dfrac{4x^2}{\sigma^2} - 2\right)e^{\frac{-x^2}{2\sigma^2}}$	$= a_2\left(\dfrac{4m\omega x^2}{\hbar} - 2\right)e^{\frac{-m\omega x^2}{2\hbar}}$

We can work out the normalisation factor a_n as a function of n. Let us first consider the first excited state. Forming and solving the normalisation integral in this case:

$$\int_{-\infty}^{\infty} {a_1}^2 \frac{4m\omega x^2}{\hbar} e^{\frac{-m\omega x^2}{\hbar}} dx = 1$$

$$2\sqrt{\frac{\pi\hbar}{m\omega}} = \frac{1}{{a_1}^2}$$

$$a_1 = \sqrt[4]{\frac{m\omega}{\hbar\pi}} \frac{1}{\sqrt{2}} = \sqrt[4]{\frac{m\omega}{\hbar\pi}} \frac{1}{\sqrt{2^1 \times 1!}}$$

Similarly, for the second excited state:

$$\int_{-\infty}^{\infty} {a_2}^2 \left(\frac{4m\omega x^2}{\hbar} - 2\right)^2 e^{\frac{-m\omega x^2}{\hbar}} dx = 1$$

$$8\sqrt{\frac{\pi\hbar}{m\omega}} = \frac{1}{{a_2}^2}$$

$$a_2 = \sqrt[4]{\frac{m\omega}{\hbar\pi}} \frac{1}{\sqrt{8}} = \sqrt[4]{\frac{m\omega}{\hbar\pi}} \frac{1}{\sqrt{2^2 \times 2!}}$$

We see a pattern emerge, whereby:

$$a_n = \sqrt[4]{\frac{m\omega}{\hbar\pi}} \frac{1}{\sqrt{2^n n!}}$$

Replacing this in the equation for the wavefunction gives us the normalised wavefunction:

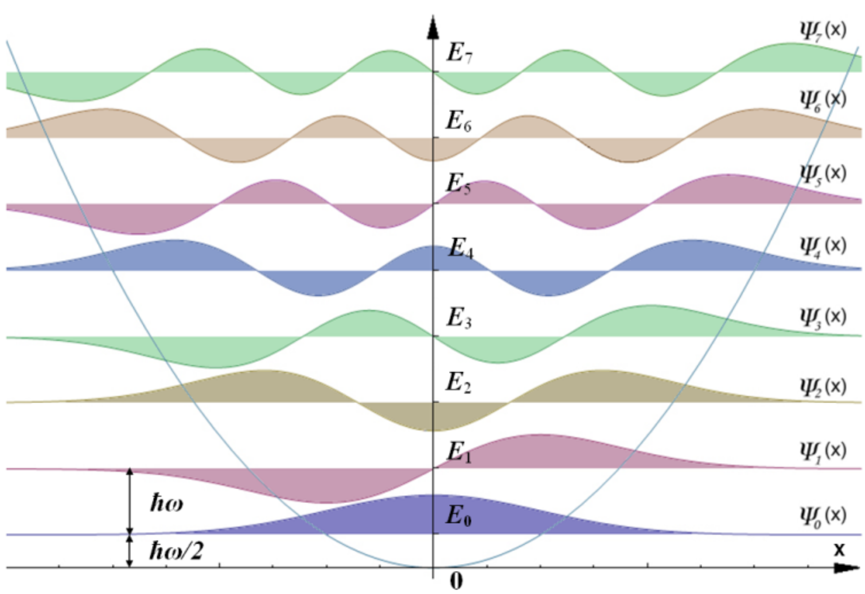
$$\boxed{\psi_n(x) = \sqrt[4]{\frac{m\omega}{\hbar\pi}} \frac{1}{\sqrt{2^n n!}} \mathrm{H}_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right) e^{\frac{-m\omega x^2}{2\hbar}}}$$

Using σ to simplify the equation:

$$\sigma = \sqrt{\frac{\hbar}{m\omega}} \Rightarrow \frac{m\omega}{\hbar\pi} = \frac{1}{\sigma^2\pi}$$

$$\boxed{\therefore \psi_n(x) = \sqrt{\frac{1}{\sigma\sqrt{\pi}}} \frac{1}{\sqrt{2^n n!}} \mathrm{H}_n\left(\frac{x}{\sigma}\right) e^{\frac{-x^2}{2\sigma^2}}}$$

To summarise, below is an illustration of the energies of the system (quantised, with equally spaced gaps of $h\omega$) and the wavefunctions:



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