Schrödinger Wave Equation

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1 The History of the Schrödinger Equation

Erwin Schrödinger published a paper on his wave equation in 1926, which later became the foundation of the theory of quantum mechanics. The Schrödinger wave equation is used to describe waves where there are significant quantum effects in some particular physical system (p. 222) [1]. It is a type of equation from the broader category of wave equations, which describe how waves propagate in space such as, for example, ocean water waves. Werner Heisenberg published a different theory explaining different types of occurrences in atoms just before Schrödinger published his paper; Schrödinger showed that they were in fact equivalent theories even though at first glance they seemed to be fairly unrelated (p. 221) [1]. Since the Schrödinger theory is easier to grasp, it will be the focus of this research report. It should also be noted that Schrödinger won the 1933 Nobel Prize in Physics for his research.

Physicists now know that particles can exhibit wave-like behaviours and that a particle's position and momentum cannot both be known exactly; the Schrödinger equation gives probability distributions but cannot predict the exact result for either. A famous example showing that a particle exhibits wave behaviour is the double-slit experiment. Electrons fired through a screen, one at a time, with two slits in it, will then hit a photosensitive detector screen behind it. Thinking of electrons as particles and not waves, we predict that we will see roughly two bright columns on the detector screen where the particles are most likely to hit. In fact, we see a spreading out pattern similar to the same experiment using water waves as a result of their interference pattern. We find bright bands alternating with dark bands, showing the places where the water waves amplify and where they cancel each other out.

We will be examining a particular system where the Schrödinger equation can be applied; this system is called the simple harmonic oscillator (p. 246) [1]. In particular, it is called the quantum harmonic oscillator system, one of the most significant models in quantum mechanics. Its significance lies partly in the fact that exact analytical solutions are known, which we will attempt to extract in the report via the power series solution method. It should be noted that usually solutions are found using the Laplace transform or by way of the Fourier transform.

2 Solutions of the Schrödinger Wave Equation

First, we start off with the one dimensional Schrödinger wave equation, which we note is the only case that it is in the form of an ordinary differential equation and not a partial differential equation (p. 227) [1]. This is due to an increase in complexity when adding more space dimensions; the wave equation must adjust to this accordingly.

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi \tag{2.1}$$

Vol. 4(1) | DOI: https://doi.org/10.31542/muse.v4i1.1317

The Schrödinger wave equation is composed of two functions both dependent on the position variable: x, $V(x)$ and $\psi = \psi(x)$. The latter is the wave function, which is the solution to the equation describing the state of a particle in the system, and the former is the potential energy function (p. 246) [1]:

$$V(x) = \frac{1}{2}\mu\omega^2 x^2 \tag{2.2}$$

After substituting the above for the potential energy, we obtain the following:

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + \frac{1}{2}\mu\omega^2 x^2\psi = E\psi \tag{2.3}$$

The latter equation is the Schrödinger wave equation for the linear harmonic oscillator, which will be the main focus of this report. We notice that this equation includes constants such as the mass μ, the total energy E, the frequency of the harmonic oscillator ω and a variant of Planck's constant $\hbar = h/2\pi$ where $h = 6.626069 \times 10^{-34} J \cdot s$ (p. 125, 161) [1]. We shall try to find solutions to this equation by first obtaining the standard form of the Schrödinger wave equation:

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + \frac{1}{2}\mu\omega^2 x^2\psi = E\psi \tag{2.4}$$

$$-\frac{\hbar^2}{2\mu}\frac{d^2\psi}{dx^2} + \frac{1}{2}\mu\omega^2 x^2\psi - E\psi = 0 \tag{2.5}$$

$$\frac{d^2\psi}{dx^2} + \frac{1}{2}\mu\omega^2 x^2\left(-\frac{2\mu}{\hbar^2}\right)\psi - E\left(-\frac{2\mu}{\hbar^2}\right)\psi = 0 \tag{2.6}$$

$$\frac{d^2\psi}{dx^2} - \frac{\mu^2\omega^2 x^2}{\hbar^2}\psi + \frac{2\mu E}{\hbar^2}\psi = 0 \tag{2.7}$$

$$\frac{d^2\psi}{dx^2} - \left(\frac{\mu^2\omega^2 x^2}{\hbar^2} - \frac{2\mu E}{\hbar^2}\right)\psi = 0 \tag{2.8}$$

Now that we have the equation in standard form, we will perform a variety of operations to transform the Schrödinger wave equation into a more useable form.

$$\frac{d^2\psi}{dx^2} = \left(\frac{\mu^2\omega^2 x^2}{\hbar^2} - \frac{2\mu E}{\hbar^2}\right)\psi \tag{2.9}$$

$$\frac{d^2\psi}{dx^2} = -\frac{\mu\omega}{\hbar}\left(\frac{2E}{\hbar\omega} - \frac{\mu\omega}{\hbar}x^2\right)\psi \tag{2.10}$$

Let $\frac{2E}{\hbar\omega} = \lambda$, allowing us to simplify our equation. After making the above substitution, we have the following:

$$\frac{d^2\psi}{dx^2} = -\frac{\mu\omega}{\hbar}\left(\lambda - \frac{\mu\omega}{\hbar}x^2\right)\psi \tag{2.11}$$

We have conveniently factored out certain values to obtain the above equation; clearly, another substitution would be beneficial. We shall change our independent variable from x to ξ, since it is more convenient to work with dimensionless variables, using the following method below. First, let us have the following, choosing the new variable to allow for significant cancellations later:

$$\xi = \sqrt{\frac{\mu\omega}{\hbar}}x \tag{2.12}$$

Now, we have that:

$$\frac{\partial\psi}{\partial\xi} = \frac{\partial\psi}{\partial x}\cdot\frac{\partial x}{\partial\xi} = \sqrt{\frac{\hbar}{\mu\omega}}\frac{\partial\psi}{\partial x} \tag{2.13}$$

As can be seen above, following partial derivative laws, we split it up into two parts where the first is with respect to x and the second is with respect to ξ. Recall that $\psi = \psi(x)$, unveiling the reason as to why we split the partial in this manner. The second partial derivative is as follows, using the same methodology:

$$\frac{\partial^2\psi}{\partial\xi^2} = \frac{\partial}{\partial\xi}\left(\sqrt{\frac{\hbar}{\mu\omega}}\frac{\partial\psi}{\partial x}\right) = \frac{\partial}{\partial x}\left(\sqrt{\frac{\hbar}{\mu\omega}}\frac{\partial\psi}{\partial x}\right)\frac{\partial x}{\partial\xi} = \sqrt{\frac{\hbar}{\mu\omega}}\frac{\partial^2\psi}{\partial x^2}\cdot\sqrt{\frac{\hbar}{\mu\omega}} = \frac{\hbar}{\mu\omega}\frac{\partial^2\psi}{\partial x^2} \tag{2.14}$$

Therefore, after rearranging, we have:

$$\frac{\partial^2\psi}{\partial\xi^2} = \frac{\hbar}{\mu\omega}\frac{\partial^2\psi}{\partial x^2} \Longrightarrow \frac{\partial^2\psi}{\partial x^2} = \frac{\mu\omega}{\hbar}\frac{\partial^2\psi}{\partial\xi^2} \tag{2.15}$$

After making the substitution for ξ and the derived second partial derivative, we obtain the following equation:

$$\frac{\mu\omega}{\hbar}\frac{d^2\psi}{d\xi^2} = -\frac{\mu\omega}{\hbar}\left(\lambda - \xi^2\right)\psi \tag{2.16}$$

$$\frac{d^2\psi}{d\xi^2} = -\left(\lambda - \xi^2\right)\psi \tag{2.17}$$

$$\frac{d^2\psi}{d\xi^2} + \left(\lambda - \xi^2\right)\psi = 0 \tag{2.18}$$

We have reduced the original equation to an easier to handle, second order ordinary differential equation, as shown above. Now, we need to find solutions to the ordinary differential equation; we will assume these solutions are of the following form:

$$\psi(\xi) = e^{-\frac{\xi^2}{2}}y(\xi) \tag{2.19}$$

Taking the derivative of this equation with respect to ξ, we obtain the following:

$$\frac{\partial\psi}{\partial\xi} = -\xi e^{-\frac{\xi^2}{2}}y(\xi) + e^{-\frac{\xi^2}{2}}y'(\xi) \tag{2.20}$$

Since we want to obtain a second order differential equation, matching the one we obtained from the Schrödinger equation, we take the derivative with respect to ξ once again, shown below:

$$\frac{\partial^2\psi}{\partial\xi^2} = -\xi e^{-\frac{\xi^2}{2}}\big(-\xi y(\xi)\big) + e^{-\frac{\xi^2}{2}}\big(-\xi y(\xi)\big)' + y'(\xi)\Big(-\xi e^{-\frac{\xi^2}{2}}\Big) + e^{-\frac{\xi^2}{2}} y''(\xi) \tag{2.21}$$

$$\frac{\partial^2\psi}{\partial\xi^2} = \xi^2 y(\xi) e^{-\frac{\xi^2}{2}} + e^{-\frac{\xi^2}{2}}\big(-y(\xi) + (-\xi) y'(\xi)\big) - \xi y'(\xi) e^{-\frac{\xi^2}{2}} + e^{-\frac{\xi^2}{2}} y''(\xi) \tag{2.22}$$

$$\frac{\partial^2\psi}{\partial\xi^2} = \xi^2 y(\xi) e^{-\frac{\xi^2}{2}} - e^{-\frac{\xi^2}{2}} y(\xi) - 2\xi y'(\xi) e^{-\frac{\xi^2}{2}} + e^{-\frac{\xi^2}{2}} y''(\xi) \tag{2.23}$$

Therefore, we have the following:

$$\frac{\partial\psi}{\partial\xi} = -\xi e^{-\frac{\xi^2}{2}} y(\xi) + e^{-\frac{\xi^2}{2}} y'(\xi) \tag{2.24}$$

and

$$\frac{\partial^2\psi}{\partial\xi^2} = \xi^2 y(\xi) e^{-\frac{\xi^2}{2}} - e^{-\frac{\xi^2}{2}} y(\xi) - 2\xi y'(\xi) e^{-\frac{\xi^2}{2}} + e^{-\frac{\xi^2}{2}} y''(\xi) \tag{2.25}$$

We will now substitute these into our second order ordinary differential equation:

$$\frac{d^2\psi}{d\xi^2} + \big(\lambda - \xi^2\big)\psi = 0 \tag{2.26}$$

$$\xi^2 y(\xi) e^{-\frac{\xi^2}{2}} - e^{-\frac{\xi^2}{2}} y(\xi) - 2\xi y'(\xi) e^{-\frac{\xi^2}{2}} + e^{-\frac{\xi^2}{2}} y''(\xi) + \big(\lambda - \xi^2\big) e^{-\frac{\xi^2}{2}} y(\xi) = 0 \tag{2.27}$$

$$e^{-\frac{\xi^2}{2}}\Big(\xi^2 y(\xi) - y(\xi) - 2\xi y'(\xi) + y''(\xi) + \big(\lambda - \xi^2\big) y(\xi)\Big) = 0 \tag{2.28}$$

We shall now divide by $e^{-\frac{\xi^2}{2}}$ and expand:

$$\xi^2 y(\xi) - y(\xi) - 2\xi y'(\xi) + y''(\xi) + \lambda y(\xi) - \xi^2 y(\xi) = 0 \tag{2.29}$$

$$y''(\xi) - 2\xi y'(\xi) + \big(\lambda - 1\big) y(\xi) = 0 \tag{2.30}$$

There are several methods for solving the Hermite equation, though, according to the literature, the most common way of tackling it is to find series solutions. First, we have the following:

$$y(\xi) = \sum_{n=0}^{\infty} a_n \xi^n \tag{2.31}$$

Since we need the derivatives of $y(\xi)$, we will take the derivative and second derivative with respect to the power series solution above, as follows:

$$y'(\xi) = \sum_{n=1}^{\infty} n a_n \xi^{n-1} \tag{2.32}$$

$$y''(\xi) = \sum_{n=2}^{\infty} n(n-1) a_n \xi^{n-2} \tag{2.33}$$

Now, we want all the indices of the sums to be the same; specifically we want all of them to start at $n = 0$. We shift the indices of $y'(\xi)$ and $y''(\xi)$ to obtain the following:

$$y'(\xi) = \sum_{n=0}^{\infty}(n+1)a_{n+1}\xi^n \tag{2.34}$$

$$y''(\xi) = \sum_{n=0}^{\infty}(n+2)(n+1)a_{n+2}\xi^n \tag{2.35}$$

We shall substitute our power series and its derivatives into our Hermite equation:

$$\sum_{n=0}^{\infty}(n+2)(n+1)a_{n+2}\xi^n - 2\xi\sum_{n=0}^{\infty}(n+1)a_{n+1}\xi^n + (\lambda-1)\sum_{n=0}^{\infty}a_n\xi^n = 0 \tag{2.36}$$

$$\sum_{n=0}^{\infty}(n+2)(n+1)a_{n+2}\xi^n - 2\sum_{n=0}^{\infty}(n+1)a_{n+1}\xi^{n+1} + (\lambda-1)\sum_{n=0}^{\infty}a_n\xi^n = 0 \tag{2.37}$$

Our middle series term has ξ^{n+1}, therefore, we will shift the index once more:

$$2\sum_{n=0}^{\infty}(n+1)a_{n+1}\xi^{n+1} \Longrightarrow 2\sum_{n=1}^{\infty}na_n\xi^n \tag{2.38}$$

Notice that we can start this series at $n = 0$ since the whole series will be equal to zero; this makes it perfect when changed in our substitution above.

$$\sum_{n=0}^{\infty}(n+2)(n+1)a_{n+2}\xi^n - 2\sum_{n=0}^{\infty}na_n\xi^n + (\lambda-1)\sum_{n=0}^{\infty}a_n\xi^n = 0 \tag{2.39}$$

$$\sum_{n=0}^{\infty}(n+2)(n+1)a_{n+2}\xi^n - 2na_n\xi^n + (\lambda-1)a_n\xi^n = 0 \tag{2.40}$$

$$\sum_{n=0}^{\infty}\big((n+2)(n+1)a_{n+2} - 2na_n + (\lambda-1)a_n\big)\xi^n = 0 \tag{2.41}$$

$$\sum_{n=0}^{\infty}\big((n+2)(n+1)a_{n+2} - \big(2n+1-\lambda\big)a_n\big)\xi^n = 0 \tag{2.42}$$

Since the whole series is equal to zero, this means that the coefficients are equal to zero:

$$(n+2)(n+1)a_{n+2} - \big(2n+1-\lambda\big)a_n \tag{2.43}$$

Hence, we obtain the following recurrence relation:

$$a_{n+2} = \frac{(2n+1-\lambda)}{(n+2)(n+1)}a_n \tag{2.44}$$

We would need to be given the values of a_0 and a_1, which respectively correspond to $y(0)$ and $y'(0)$. Note that $y(0)$ corresponds to the particle's displacement and $y'(0)$ corresponds to the particle's velocity. This power series would become an infinite polynomial, as n becomes arbitrarily large and would be a divergent series. We can see it is divergent by comparing it to the series of e^{u^2}, whose coefficients behave exactly like those in our own series, as we will see below.

$$e^{z^2} = \sum_{k=0}^{\infty} \frac{(z^2)^k}{k!} = \sum_{k=0}^{\infty} \frac{z^{2k}}{k!} \tag{2.45}$$

Let $n = 2k$, then we have:

$$e^{z^2} = \sum_{k=0}^{\infty} \frac{z^{2k}}{k!} = \sum_{n=0,2,4,\dots}^{\infty} \frac{z^n}{\left(\frac{n}{2}\right)!} \tag{2.46}$$

Check the coefficients of this series as follows, when $n \to \infty$:

$$\frac{c_{n+2}}{c_n} = \frac{\left(\frac{n}{2}\right)!}{\left(\frac{n+2}{2}\right)!} = \frac{1}{\frac{n}{2}+1} = \frac{2}{n\left(1+\frac{2}{n}\right)} \approx \frac{2}{n} \Longrightarrow c_{n+2} \approx \frac{2}{n}c_n;\ n \in \{0,1,2,\dots\} \tag{2.47}$$

Therefore, we can see from the recursion relation of our original series that as $n \to \infty$, we have:

$$a_{n+2} = \frac{(2n+1-\lambda)}{(n+2)(n+1)}a_n \Longrightarrow a_{n+2} \approx \frac{2}{n}a_n;\ n \in \{0,1,2,\dots\} \tag{2.48}$$

We do not want to obtain an infinite polynomial and therefore want the series to terminate beyond a given n. First, recall that $\lambda = \frac{2E}{\hbar\omega}$. Then, if for some specific total energy E, we can get λ to be an odd integer such that $2n+1-\lambda$ in the numerator of our recursion relation is zero, we can terminate the series since all coefficients after will be zero as well.

$$2n+1-\lambda = 0 \Longrightarrow \lambda = 2n+1 \Longrightarrow \frac{2E}{\hbar\omega} = 2n+1 \Longrightarrow E_n = \hbar\omega\left(n+\frac{1}{2}\right);\ n \in \{0,1,2,\dots\} \tag{2.49}$$

Therefore, we have the total energy at the n^{th} energy level, where $n = 0$ is the ground state and $n \geq 1$ are excited states (p. 247) [1]. It is important to note that the energies are very specific values at each energy level; in other words, they are quantized (p. 247) [1]. Physicists call the power series solutions obtained above Hermite polynomials denoted $y(\xi) = H_n(\xi)$ (p. 248) [1]. Therefore, our coefficient a_n will be the last nonzero term before the series terminates, since $a_{n+2} = 0$, and so we can write our solution in the form of a finite polynomial:

$$H_n(\xi) = y(\xi) = a_n\xi^n + a_{n-2}\xi^{n-2} + \cdots;\ n \in \{0,1,2,\dots\} \tag{2.50}$$

and this Hermite polynomial is the solution to the equation:

$$y''(\xi) - 2\xi y'(\xi) + \left(\lambda - 1\right)y(\xi) = 0 \tag{2.51}$$

Of course, this solution depends on whether we are using the recursion relation starting with a_0 giving the even solution, or a_1 giving the odd solution.

Hence, we have that our solutions to the second order differential equation:

$$\frac{d^2\psi}{d\xi^2} + \left(\lambda - \xi^2\right)\psi = 0 \tag{2.52}$$

are as follows:

$$\psi(\xi) = e^{-\frac{\xi^2}{2}} y(\xi) \Longrightarrow \psi_n(\xi) = A_n e^{-\frac{\xi^2}{2}} H_n(\xi);\ n \in \{0, 1, 2, \ldots\} \tag{2.53}$$

where A_n are normalization constants and the $H_n(\xi)$ are the Hermite polynomials, which we will not explicitly write out here.

We need to back substitute to find our solution to our original Schrödinger wave equation in terms of $\psi(x)$, as shown below:

$$\psi_n(x) = c_n e^{-\frac{\sqrt{\frac{\mu\omega}{\hbar}}^2 x^2}{2}} H_n\left(\sqrt{\frac{\mu\omega}{\hbar}} x\right);\ n \in \{0, 1, 2, \ldots\} \tag{2.54}$$

$$\psi_n(x) = c_n e^{-\frac{\mu\omega}{2\hbar} x^2} H_n\left(\sqrt{\frac{\mu\omega}{\hbar}} x\right);\ n \in \{0, 1, 2, \ldots\} \tag{2.55}$$

These are called the wave functions, or eigenfunctions, of the harmonic oscillator system and they satisfy the conditions (p. 228) [1]:

$$\psi \to 0 \text{ as } |x| \to \infty \tag{2.56}$$

$$\int_{-\infty}^{\infty} \left|\psi(x)\right|^2\, dx = 1 \tag{2.57}$$

for the specific total energy levels that we found, shown below:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right);\ n \in \{0, 1, 2, \ldots\} \tag{2.58}$$

References

[1] Paul A. Tipler and Ralph A. Llewellyn. *Modern Physics*. W.H. Freeman and Company. Fifth Edition, 2008. Pages 125, 161, 221 - 248. Print.