4 Solutions of the 1D Schrödinger equation

We now look at various examples of solutions to the 1D SE for one particle:

4.1 Example I: Stationary states

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)+V(x)\psi(x,t)=i\hbar\frac{\partial}{\partial t}\psi(x,t)\,. \tag{4.1}$$

Assume V is time-independent. We can then use the method of *separation of variables* to find solutions, by trying the ansatz

$$\psi(x,t)=\psi(x)T(t)\,. \tag{4.2}$$

This gives us

$$(\hat{H}\psi(x))T(t)=\psi(x)(i\hbar\frac{\partial}{\partial t}T(t))\,, \tag{4.3}$$

and so

$$\frac{1}{\psi(x)}\hat{H}\psi(x)=\frac{1}{T(t)}(i\hbar\frac{\partial}{\partial t}T(t))\,. \tag{4.4}$$

Since the left hand side depends only on x and the right hand side only on t, both must equal a constant, which we call E. We thus have

$$T(t)=\exp(\frac{-i}{\hbar}Et)\,. \tag{4.5}$$

and the *time-independent Schrödinger equation*

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+V(x)\psi(x)=E\psi(x)\,. \tag{4.6}$$

Solutions to the SE of the form

$$\psi(x)\exp(\frac{-i}{\hbar}Et),$$

where $\psi(x)$ is a solution to (4.6) are called *stationary states.*

We say $\psi(x)$ is an *eigenfunction* of the hamiltonian operator $\hat{H}$ which corresponds to a physical state whose energy is given by the *eigenvalue* E. When $V=0$, (4.6) reduces to

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)=E\psi(x)\,. \tag{4.7}$$

More generally, if

$$A\psi(x)=a\psi(x) \tag{4.8}$$

for some operator A and complex number a, then we say $\psi(x)$ is an *eigenfunction* of A with *eigenvalue* a. The terminology is a natural extension to infinite-dimensional spaces (of functions) of the definitions of eigenvector and eigenvalue for finite-dimensional matrices: compare the eigenequation $Av = av$ for matrix A, vector v and complex number a.

As we will see, the eigenvalues of physically significant operators are observable physical quantities. They turn out always to be real – as we would expect, since we know of no natural way to directly observe a complex number in nature. We will see the mathematical reason for this when we discuss the general formalism of quantum mechanics.

Notes

- Equation (4.7) has solution $e^{i(kx-\omega t)}$, where $E = \frac{\hbar^2 k^2}{2m} = \hbar\omega$. This is the de Broglie wave we originally considered, so our discussion is at least self-consistent.

- This de Broglie wave solution to the 1D SE for a free particle is *not* normalisable, and so does not have a well-defined probabilistic interpretation via the Born rule. The quantum mechanical free particle is a very useful idealisation, but not a physical solution. We never actually have a uniformly zero potential throughout space, nor a single particle whose wavefunction is spread uniformly over all of space. There could not be any consistent way of assigning probabilities to finding such a particle in finite regions, since there is no well-defined uniform probability distribution on the 1D real line. (The same is true in 3D, of course.)

- Any stationary state $\psi(x,t) = \psi(x)e^{-\frac{iEt}{\hbar}}$ has probability density

  $$\rho(x,t) = |\psi(x,t)|^2 = |\psi(x)|^2 \,.$$

  In other words, its probability density is time-independent. More generally, we will see the probability of measuring any given outcome for any dynamical quantity is time-independent. Hence the name *stationary* state.

4.2 Completeness of the energy eigenfunctions

An important fact is that the general solution to the SE with t-independent potential $V(x)$ is a *superposition* of stationary states:

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}} \,. \tag{4.9}$$

This follows from the fact that any wavefunction at a given time, say $t = 0$, can be written as a superposition of energy eigenfunctions, so that,

$$\psi(x,0) = \sum_{n=1}^{\infty} a_n \psi_n(x) \,, \tag{4.10}$$

and from the linearity of the SE.

We will see later (from theorem 6.3) that Eqn. (4.10) is a special case of the more general result that any wavefunction can be written as a superposition of eigenfunctions for any operator corresponding to a physically observable quantity.

If the set of energy eigenvalues is continuous, we need to replace the sum by an integral. If there are continuous and discrete subsets, we need both sum and integral. Thus if there is a discrete set of normalised energy eigenfunctions $\{\psi_i\}_{i=1}^N$ (we include $N = \infty$ as a possibility) and a continuous set of eigenfunctions $\{\psi_\alpha\}_{\alpha\in\Delta}$, where the indexing set Δ is some sub-interval of the real numbers, we can write

$$\psi(x,t) = \sum_{n=1}^{N} a_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}} + \int_\Delta a_\alpha \psi_\alpha(x) e^{-\frac{iE_\alpha t}{\hbar}} d\alpha\,, \tag{4.11}$$

4.3 Example II: Gaussian wavepackets

As an example of a continuous superposition of free particle stationary states, consider

$$\psi(x,t) = C\int_{-\infty}^{\infty} e^{-\frac{\sigma}{2}(k-k_0)^2} e^{i(kx-\frac{\hbar k^2}{2m}t)}dk\,. \tag{4.12}$$

The exponent here is $-\frac{1}{2}(\sigma+\frac{i\hbar t}{m})k^2+(k_0\sigma+ix)k-\frac{\sigma}{2}k_0^2$, which we can write in the form $-\frac{1}{2}a(k-\frac{b}{a})^2+(\frac{b^2}{2a}-\frac{\sigma}{2}k_0^2)$, where $a=\sigma+\frac{i\hbar t}{m}$, $b=k_0\sigma+ix$.

Now we have

$$\int e^{-\frac{1}{2}a(k-\frac{b}{a})^2}dk = \sqrt{\frac{2\pi}{a}}\,. \tag{4.13}$$

This gives us

$$\psi(x,t) = C'\sqrt{\frac{2\pi}{\sigma+\frac{i\hbar t}{m}}}\exp(\frac{(k_0\sigma+ix)^2}{2(\sigma+\frac{i\hbar t}{m})}) \tag{4.14}$$

$$\begin{aligned}|\psi(x,t)|^2 &= C''\sqrt{\frac{1}{\sigma^2+\frac{\hbar^2t^2}{m^2}}}\exp(\frac{(k_0\sigma+ix)^2}{2(\sigma+\frac{i\hbar t}{m})}+\frac{(k_0\sigma-ix)^2}{2(\sigma-\frac{i\hbar t}{m})})\\ &= C''\sqrt{\frac{1}{\sigma^2+\frac{\hbar^2t^2}{m^2}}}\exp(\frac{\sigma^3k_0^2-\sigma x^2+\frac{2k_0\sigma x\hbar t}{m}}{\sigma^2+\frac{\hbar^2t^2}{m^2}})\\ &= C'''\sqrt{\frac{1}{\sigma^2+\frac{\hbar^2t^2}{m^2}}}\exp(\frac{-\sigma(x-\frac{k_0\hbar t}{m})^2}{\sigma^2+\frac{\hbar^2t^2}{m^2}})\qquad,\end{aligned} \tag{4.15}$$

where C', C'' and C''' are constants.

Since

$$\begin{aligned}\int_{-\infty}^{\infty}|\psi(x,t)|^2dx &= C'''\sqrt{\frac{2(\sigma^2+\frac{\hbar^2t^2}{m^2})\pi}{2\sigma}}\sqrt{\frac{1}{(\sigma^2+\frac{\hbar^2t^2}{m^2})}}\\ &= C'''\sqrt{\frac{\pi}{\sigma}}\end{aligned} \tag{4.16}$$

the normalisation condition gives us

$$C''' = \sqrt{\frac{\sigma}{\pi}}\,. \tag{4.17}$$

Notes:

- The Gaussian wavepacket describes an *approximately localised* particle, almost all of whose probability density is within a finite region of size $\approx N(\sigma^2 +$

$\frac{\hbar^2 t^2}{m^2})^{\frac{1}{2}}\sigma^{-\frac{1}{2}}$ at time t, for some smallish positive number N.[12] This follows since the probability density function is a Gaussian curve with standard deviation $(\sigma^2 + \frac{\hbar^2 t^2}{m^2})^{\frac{1}{2}}\sigma^{-\frac{1}{2}}$.

- Recall that we obtained the Gaussian wavepacket as a superposition of stationary states. Considering its evolution, we thus see that a superposition of stationary states is *not* necessarily stationary, since the Gaussian wavepacket's probability density function varies with time.

- From Eqn. (4.15), we see the speed of the Gaussian wavepacket's centre is $\approx \frac{\hbar k_0}{m}$. Since its standard deviation is

  $$(\sigma^2 + \frac{\hbar^2 t^2}{m^2})^{\frac{1}{2}}\sigma^{-\frac{1}{2}} \approx \frac{\hbar t}{m\sigma^{\frac{1}{2}}} \tag{4.18}$$

  for large t, the speed at which it spreads in width is $\approx \frac{\hbar}{m\sigma^{\frac{1}{2}}}$. Note that, mathematically speaking, neither is necessarily bounded by the speed of light c. This illustrates that the Schrödinger equation is *non-relativistic* – i.e. incompatible with special relativity. If it was possible to produce Gaussian wavepackets for any values of k_0 and σ, and if the Schrödinger equation precisely described their evolution, we could use the wavepackets to send signals faster than light.[13]

  As this suggests, the SE is only approximately valid. [14] We cannot use Gaussian wavepackets (or, unless we find experimental evidence against special relativity, anything else) to send signals faster than light. However, the SE is a good enough approximation to allow us to understand a great deal of physics and chemistry.

- Pictures of an evolving Gaussian wave packet can be found at (for example) http://demonstrations.wolfram.com/EvolutionOfAGaussianWavePacket/

4.4 Example III: Particle in an infinite square potential well

Consider a particle confined by a 1D box with impermeable walls. We can model this by a potential

$$V(x) = \begin{cases} 0 & |x| < a\,, \\ \infty & |x| > a\,. \end{cases} \tag{4.19}$$

We look for stationary states obeying

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)\,, \tag{4.20}$$

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[12] For example, 99.7% of the probability density is within the region defined by $N = 3$.

[13] We can also see that the SE is non-relativistic by noting that it is second order in x and first order in t. A relativistically invariant equation must be of the same order in x and t, because Lorentz transformations map x and t to linear combinations.

[14] Quantum mechanics, which is the topic of this course, is a non-relativistic theory, which is approximately correct when relativistic corrections are small. Physicists tend to think of quantum theory as defining a mathematical framework, and non-relativistic quantum mechanics as a particular theory within this framework. The framework of quantum theory also includes relativistic quantum field theories, which (as the name suggests) *are* consistent with special relativity. In particular, there is a relativistically invariant equation for the evolution of an electron's wavefunction, from which the SE emerges as a non-relativistic limit. We won't worry about relativistic corrections or extensions of quantum mechanics in this course; they are discussed in Part III.

which gives us

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = \begin{cases} E\psi(x) & |x| < a\,, \\ (E-\infty)\psi(x) & |x| > a\,. \end{cases} \tag{4.21}$$

Here the second alternative is a useful but unrigorous shorthand, and should perhaps be written in quotation marks to emphasize this. The next paragraph explains how we handle the infinity.

4.4.1 Handling discontinuities

We need a consistent treatment of discontinuities in $V(x)$ and (hence perhaps) in $\psi(x)$, $\frac{d\psi}{dx}, \ldots$. One method is to take a discontinuous $V(x)$ as the limiting case of a set of continuous potentials, and consider the limits of the solutions $\psi(x)$. But we can address the SE with discontinuous $V(x)$ directly using the following rules:

A step function discontinuity in ψ would create a delta function derivative in $\frac{d^2\psi}{dx^2}$ on the LHS of the SE, which would not be cancelled by other terms. So we expect ψ to be continuous everywhere.

A step function discontinuity in $\frac{d\psi}{dx}$ would create a delta function in $\frac{d^2\psi}{dx^2}$ on the LHS of the SE; we can allow this only at points where $V(x)$ is infinitely discontinuous.

A step function discontinuity in $\frac{d^2\psi}{dx^2}$ gives a step function discontinuity on the LHS of the SE; we can allow this only at points where $V(x)$ has a finite step function discontinuity so that the two discontinuities on the LHS cancel.

So, for the infinite square well we expect ψ to be continuous everywhere, and $\frac{d\psi}{dx}$ to be continuous except at $|x| = a$. Since $V = \infty$ for $|x| > a$, we need $\psi = 0$ in this region for consistency of the SE. We have

$$\psi(x) = A\cos(kx) + B\sin(kx)\,, \qquad k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \text{in } |x| < a\,. \tag{4.22}$$

Now $\psi = 0$ at $x = \pm a$ gives

$$A\cos(ka) \pm B\sin(ka) = 0 \tag{4.23}$$

and hence

$$A\cos(ka) = 0 \text{ and } B\sin(ka) = 0\,. \tag{4.24}$$

Hence

$$\begin{aligned}
&\underline{\text{either}}\ A = 0\,, && \sin(ka) = 0\,, \\
&\qquad \psi(x) = B\sin(kx)\,, && k = \frac{n\pi}{2a}\ \text{for}\ n \geq 2\ \text{even}\,. \\
&\underline{\text{or}}\ B = 0\,, && \cos(ka) = 0\,, \\
&\qquad \psi(x) = A\cos(kx)\,, && k = \frac{n\pi}{2a}\ \text{for}\ n \geq 1\ \text{odd}\,.
\end{aligned} \tag{4.25}$$

This gives us solutions for

$$E = E_n = \frac{\hbar^2\pi^2 n^2}{8ma^2}\ \text{for}\ n = 1, 2, 3, \ldots \tag{4.26}$$

Notes:

- We have *quantised* (i.e. discrete) energies for the stationary states of the infinite square well. Cf. the Bohr atom – it begins to look plausible that quantum mechanics could explain the apparent quantisation of physical states. Perhaps the allowed electron orbits in the Bohr atom correspond to the stationary states in a 3D Coulomb potential?[15]

- The solutions fall into two classes:

$$\psi(x) = \begin{cases} \psi(-x) & \underline{\text{even}}\ \text{parity}\,, \\ -\psi(-x) & \underline{\text{odd}}\ \text{parity}\,. \end{cases} \tag{4.27}$$

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[15] We will see later that the relationship is a bit more complicated, but the intuition is along the right lines.

4.5 Parity

Let us consider this last phenomenon more generally. Suppose that $V(x) = V(-x)$ and that $\psi(x)$ is a solution of the time-independent SE. We have

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

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

obtaining the second equation by substituting $y = -x$ in the first. Hence $\psi(-x)$ is *also* a solution of the time-independent SE.

There are two possibilities:
(i) $\psi(x)$ and $\psi(-x)$ are linearly independent. Then $\psi(x) + \psi(-x)$ and $\psi(x) - \psi(-x)$ are also linearly independent, and have parity $+1$ and -1 respectively.
(ii) $\psi(x)$ and $\psi(-x)$ are linearly dependent: $\psi(-x) = A\psi(x)$. Then

$$\psi(x) = A\psi(-x) = A^2\psi(x) \tag{4.28}$$

so we have

$$A = \pm 1\,. \tag{4.29}$$

$A = 1$ implies $\psi(x) = \psi(-x)$, so ψ has even parity. $A = -1$ implies $\psi(x) = -\psi(-x)$, so ψ has odd parity.

Conclusion Any solution of the t-independent SE with a symmetric potential is a linear combination of solutions of definite parity.[16]

4.6 Example IV: Particle in a finite square well

A slightly more realistic model of a confined particle is given by the finite square well potential

$$V(x) = \begin{cases} -U & |x| < a\,, \\ 0 & |x| > a\,. \end{cases} \tag{4.30}$$

– a crude model of the Coulomb potential of a charged nucleus. We will look for *bound state* solutions – normalisable solutions – as opposed to unnormalisable *scattering solutions*, whose physical interpretation we will discuss later.

A solution of energy E obeys

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = \begin{cases} (E+U)\psi(x) & |x| < a\,, \\ E\psi(x) & |x| > a\,. \end{cases} \tag{4.31}$$

If $E > 0$, the solution for $|x| > a$ takes the form $\psi = Ae^{ikx} + Be^{-ikx}$, where $k^2 = \frac{2mE}{\hbar}$. This is unnormalisable.

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[16] One can also prove that the ground state (lowest energy solution), if one exists, is unique and has even parity. In fact, one can prove the stronger result that the ground state wavefunction is unique, real and strictly positive, which implies that it must have even parity. See for example, volume 4 of Reed and Simon, "Methods of Modern Mathematical Physics", Theorem XIII.4.6. A proof is also given in Eugene Lim's lecture notes for an earlier version of this course, available online.

So we require $E < 0$. We will assume that $E > -U$, i.e. that $|E| < U$, since we do not expect there to be solutions with energy lower than the minimum potential.

Exercise: Verify that indeed there are no such solutions.

Let

$$k^2 = \frac{2m|E|}{\hbar^2}\,, \tag{4.32}$$

$$l^2 = \frac{2m(U - |E|)}{\hbar^2}\,, \tag{4.33}$$

$$\text{so that} \quad k^2 + l^2 = \frac{2mU}{\hbar^2}\,. \tag{4.34}$$

For $|x| > a$ we have

$$\psi(x) = Ae^{-kx} + Be^{kx}\,, \tag{4.35}$$

and normalisability implies that

$$\psi(x) = \begin{cases} Ae^{-kx} & x > a\,, \\ Be^{kx} & x < -a\,. \end{cases} \tag{4.36}$$

For $|x| < a$ we have

$$\psi(x) = C\cos(lx) + D\sin(lx)\,. \tag{4.37}$$

Since we know that the states of definite parity span the space of all bound states, we can solve separately for even and odd parity states to get a complete spanning set of solutions.

Consider the even parity solutions. If $\psi(x) = \psi(-x)$ we have:

$$\psi(x) = \begin{cases} Ae^{-kx} & x > a\,, \\ Ae^{kx} & x < -a\,, \\ C\cos(lx) & |x| < a. \end{cases} \tag{4.38}$$

$$\psi'(x) = \begin{cases} -kAe^{-kx} & x > a\,, \\ Ake^{kx} & x < -a\,, \\ -lC\sin(lx) & |x| < a. \end{cases} \tag{4.39}$$

As ψ and ψ' are continuous at $x = \pm a$, we find

$$C\cos(la) = A\exp(-ka)\,, \tag{4.40}$$

$$-lC\sin(la) = -kA\exp(-ka)\,. \tag{4.41}$$

This gives

$$k = l\tan(la)$$

or

$$(ka) = (la)\tan(la) \tag{4.42}$$

and from (4.34) we have

$$(ka)^2 + (la)^2 = \frac{2mUa^2}{\hbar^2}\,. \tag{4.43}$$

We can solve these last two equations graphically.

The odd parity bound states (if any exist) can be similarly obtained.

The finite square well illustrates a general feature of quantum potentials $V(x)$ such that $V(x) \to 0$ as $x \to \pm\infty$. The time-independent SE has two linearly independent solutions.

For $E > 0$, these take the form of scattering solutions

$$\begin{aligned}\psi(x) &= A\exp(ikx) + B\exp(-ikx) \text{ as } x \to -\infty\\ &\quad C(A,B)\exp(ikx) + D(A,B)\exp(-ikx) \text{ as } x \to \infty\,.\end{aligned}$$

For $E < 0$, they have the form

$$\begin{aligned}\psi(x) &= A\exp(kx) + B\exp(-kx) \text{ as } x \to -\infty\\ &\quad C(A,B)\exp(kx) + D(A,B)\exp(-kx) \text{ as } x \to \infty\,.\end{aligned}$$

Here $C(A,B)$ and $D(A,B)$ are linear in A and B, and depend also on k and on the parameters defining $V(x)$.

Only for special values of $E < 0$ can we find solutions such that $B = 0$ and $C(A,B) = 0$, as required for normalisability. For the remaining values of $E < 0$, the solutions blow up exponentially as $x \to -\infty$ or as $x \to \infty$ (or both) and are unphysical: neither bound states nor scattering solutions.

[These asymptotically exponential functions are not physically meaningful: they are not normalisable and do not define eigenfunctions of $\hat{H}$.]

4.7 Example V: The quantum harmonic oscillator

has potential

$$V(x) = \frac{1}{2} m \omega^2 x^2 \,. \tag{4.44}$$

This is a particularly important example for several reasons.

First, it is not only solvable but (as we will see later) has a very elegant solution that explains some important features of quantum theory.

Second, generic symmetric potentials in 1D are at least approximately described by Eqn. (4.44). To see this, consider a potential $V(x)$ taking a minimum value V_{min} at x_{min} and symmetric about x_{min}. Writing $y = x - x_{\mathrm{min}}$, we have

$$\begin{aligned} V(y) &= V(0) + yV'(0) + \frac{y^2}{2!}V''(0) + \frac{y^3}{3!}V'''(0) + \dots \\ &\approx V_{\mathrm{min}} + \frac{y^2}{2!}V''(0) + O(y^4) \,. \end{aligned}$$

Renormalising the potential so that $V_{\mathrm{min}} = 0$, and taking $V''(0) = m\omega^2$, we recover (4.44). (If $V''(0) = 0$ this argument does not hold, but even in this case the harmonic oscillator potential can be a good qualitative fit. See for example comments below on approximating a finite square well potential by a harmonic oscillator potential.)

In fact, we can show something more general. Suppose we have a system with n degrees of freedom that has a unique stable equilibrium. Then the small oscillations about equilibrium can be approximated by n independent harmonic oscillators. This means that solving the harmonic oscillator allows us to give a quantum description of molecules excited by radiation (and hence understand the greenhouse effect and many other phenomena) and of the behaviour of crystals and other solids.

Third, the harmonic oscillator plays an even more fundamental role in quantum field theory, where we understand particles as essentially harmonic oscillator excitations of fields. Our entire understanding of matter and radiation is thus based on the quantum harmonic oscillator!

To obtain the stationary states of the quantum harmonic oscillator we need to solve

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + \frac{1}{2}m\omega^2 x^2 \psi(x) = E\psi(x) \,. \tag{4.45}$$

We define

$$y = \sqrt{\frac{m\omega}{\hbar}}\, x \text{ and } \alpha = \frac{2E}{\hbar\omega} \,. \tag{4.46}$$

We have

$$\frac{d^2\psi}{dy^2} - y^2\psi = -\alpha\psi \,. \tag{4.47}$$

If $\psi \sim \exp(-\frac{1}{2}y^2)$, then $\psi' \sim -y\exp(-\frac{1}{2}y^2)$ and $\psi'' \sim y^2\exp(-\frac{1}{2}y^2)$ to leading order, which means that $\psi'' - y^2\psi \sim (y^2 - y^2)\exp(-\frac{1}{2}y^2)$ satisfies (4.47) to leading order. Similarly $\psi \sim y^n \exp(-\frac{1}{2}y^2)$ satisfies (4.47) to leading order. This suggests considering power series solutions of the form

$$\psi(y) = H(y)e^{-\frac{y^2}{2}}\,, \tag{4.48}$$

$$H(y) = \sum_{m=0}^{\infty} a_m y^m\,, \tag{4.49}$$

and trying to match the coefficients a_m to produce an exact solution.

From (4.47) we get

$$\psi'' + (\alpha - y^2)\psi = 0 \tag{4.50}$$

and substituting from (4.48, 4.50) we get

$$\frac{d^2}{dy^2}(H\exp(-\frac{y^2}{2})) + (\alpha - y^2)H\exp(-\frac{y^2}{2}) = 0 \tag{4.51}$$

$$(H'' - 2yH' + Hy^2 - H + (\alpha - y^2)H)\exp(-\frac{y^2}{2}) = 0 \tag{4.52}$$

$$(H'' - 2yH' + (\alpha - 1)H)\exp(-\frac{y^2}{2}) = 0 \tag{4.53}$$

We have

$$H'(y) = \sum_{m=0}^{\infty} m a_m y^{m-1}\,, \tag{4.54}$$

$$\begin{aligned} H''(y) &= \sum_{m=0}^{\infty} m(m-1)a_m y^{m-2} \\ &= \sum_{m=0}^{\infty} a_{m+2}(m+2)(m+1)y^m\,. \end{aligned} \tag{4.55}$$

So from (4.53) we get

$$\sum_{m=0}^{\infty}(a_{m+2}(m+2)(m+1) - a_m(2m+1-\alpha))y^m = 0\,. \tag{4.56}$$

This must be true for all y, so each coefficient of y^m must vanish:

$$a_{m+2} = \frac{(2m+1-\alpha)}{(m+2)(m+1)}a_m \text{ for } m = 0, 1, 2, \ldots\ . \tag{4.57}$$

which determines the a_m for $m \geq 2$ in terms of a_0 and a_1.

For large m, (4.57) gives $a_{m+2} \approx \frac{2}{m} a_m$, which asymptotically describes the coefficients of e^{y^2}:

$$e^{y^2} = \sum_{n=0}^{\infty} \frac{1}{n!} y^{2n} = \sum_{n=0}^{\infty} b_n y^n \tag{4.58}$$

where for n odd we have $b_n = 0$ and for n even we have

$$b_{n+2} = \frac{1}{\frac{n}{2}+1} b_n = \frac{2}{n+2} b_n \approx \frac{2}{n} b_n \, . \tag{4.59}$$

So, if the power series is infinite, we expect

$$H(y) \approx C e^{y^2}$$

for some nonzero constant C: i.e. that $\frac{H(y)}{Ce^{y^2}} \to 1$ as $y \to \infty$. This implies that

$$\psi(y) \approx H(y) e^{-\frac{y^2}{2}} \approx C e^{\frac{1}{2} y^2} \, , \tag{4.60}$$

which is not normalisable.

We can justify this rigorously by noting that, for any $\epsilon > 0$, there exists some integer m_0 such that for all $m \geq m_0$ we have

$$\frac{a_{m+2}}{a_m} > \frac{2(1-\epsilon)}{m} \, . \tag{4.61}$$

Hence we have that

$$H(y) > C e^{(1-\epsilon) y^2} - P(y) \, , \tag{4.62}$$

where $C = a_{m_0} \neq 0$ and $P(y)$ is a polynomial of degree $\leq m_0$. This implies that there exists a y_0 such that for all $y \geq y_0$ we have

$$|H(y)| > \frac{C}{2} e^{(1-\epsilon) y^2} \, , \tag{4.63}$$

and hence

$$|\psi(y)| > \frac{C}{2} e^{(\frac{1}{2}-\epsilon) y^2} \, . \tag{4.64}$$

So indeed $\psi(y)$ diverges as $y \to \infty$, and in particular ψ is not normalisable.

We thus need the power series to be truncated to a polynomial in order to find normalisable physical solutions. Again, we can consider fixed (even and odd) parity solutions separately:

- Even parity: $a_0 \neq 0$, $a_1 = 0$, $\alpha = 2m + 1$ for some even m.
- Odd parity: $a_0 = 0$, $a_1 \neq 0$, $\alpha = 2m + 1$ for some odd m.

So the physical solutions are given by

$$\alpha = \frac{2E}{\hbar\omega} = 2m + 1 \qquad (m = 0, 1, 2, \ldots) \tag{4.65}$$

i.e.

$$E = (m + \frac{1}{2})\hbar\omega \qquad (m = 0, 1, 2, \ldots)\,. \tag{4.66}$$

The harmonic oscillator has energy levels equally spaced, separated by $\hbar\omega$, with minimum (or *zero-point*) energy $\frac{1}{2}\hbar\omega$.

The polynomials $H_n(y)$ corresponding to the physical solutions with energy $(n+\frac{1}{2})\hbar\omega$ are the *Hermite polynomials* of degree n. We can obtain them explicitly[17] from (4.65), using conventional normalisations:

$$H_0 = 1\,, H_1 = 2y\,, H_2 = 4y^2 - 2\,, H_3 = 8y^3 - 12y\,, \ldots\,. \tag{4.67}$$

The corresponding wavefunctions are thus (up to normalisation)

$$\psi_0 = e^{-\frac{1}{2}y^2}\,, \psi_1 = 2ye^{-\frac{1}{2}y^2}\,, \ldots \tag{4.68}$$

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[17] In fact one can derive a general expression (see e.g. Schiff, "Quantum Mechanics", 3rd edition):

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2}\,.$$