THE HARMONIC OSCILLATOR.

The Simple Harmonic Oscillator in classical mechanics has restoring force proportional to displacement, $F = -kx$, where k is, [1] for example, the elastic constant of a spring from which a mass, m is suspended. The corresponding time-independent potential is $V(x) = \frac{1}{2}kx^2$. The *classical solution* to Newton's equation of motion is of the form $x(t) = A\cos(\omega_0 t) + B\sin(\omega_0 t)$, where the angular frequency is $\omega_0 = \sqrt{\frac{k}{m}}$. We usually express the potential in terms of this frequency:

$$V(x) = \frac{1}{2}m\omega_0^2 x^2 \tag{1}$$

The corresponding Quantum Harmonic Oscillator thus corresponds to a Hamiltonian,

$$\widehat{H}(x) = \frac{\widehat{p}^2}{2m} + \frac{1}{2}m\omega_0^2 x^2, \tag{2}$$

with the TISE being $\widehat{H}\psi(x) = E\psi(x)$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega_0^2 x^2\psi(x) = E\psi(x). \tag{3}$$

This equation can be solved by first simplifying with a change to the dimensionless variables ξ and ϵ,

$$\xi \equiv \beta x \quad \text{where} \quad \beta \equiv \left(\frac{m\omega_0}{\hbar}\right)^{\frac{1}{2}}, \tag{4}$$

$$\text{and} \quad E = \frac{1}{2}\hbar\omega_0\epsilon, \tag{5}$$

leading to

$$\frac{d^2\psi}{d\xi^2} + (\epsilon - \xi^2)\psi = 0. \tag{6}$$

This equation may then be cast into a standard one first studied by the mathematician Hermite by making the substitution, [2]

$$\begin{aligned}\psi(x) &= H(\xi)e^{-\frac{1}{2}\xi^2} \\ &= H(\beta x)e^{-\frac{1}{2}\beta^2 x^2},\end{aligned} \tag{7}$$

where $H(\xi)$ is *not* the Hamiltonian, but a set of functions known as Hermite polynomials. They satisfy the Hermite equation obtained from making the above substitution into the TISE:

$$\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (\epsilon - 1)H = 0. \tag{8}$$

This equation is no more mysterious than the familiar equation whose most general solution is a linear combination of sines and cosines:

$$\frac{d^2\psi}{dx^2} + \omega^2 x^2\psi = 0. \tag{9}$$

If we had not yet met sines and cosines we could 'discover' them by solving this equation: the technique, Fredholm's, is to try a solution in the form of an infinite power series with undetermined coefficients:

$$\psi(x) = \sum_{n=1}^{\infty} a_n x^{n+k} \tag{10}$$

[1] This was denoted s in the first year course on Vibrations & Waves.

[2] We explain the motivation for this substitution in Appendix F.

Substitution into the equation then determines allowed values for the parameter k as well as the form of the coefficients a_n. For the latter equation we find two possible solutions ($k = 0, 1$) which turn out to be the familiar Taylor series for cos and sin. The method also works for the Hermite equation, but with a new twist. For arbitrary ϵ neither solution is physically admissible because they increase exponentially (e^{ξ^2}) at large distance, violating the requirement that the wave function vanish at infinity. However, for the special values, $\epsilon = (2n+1), \qquad n = 0, 1, 2, \ldots$, corresponding to a quantised energy, the series *terminate* at the n-th term. By becoming finite series they are merely polynomials and therefore avoid the bad exponentially increasing behaviour at infinity. This is how the energy quantisation comes about in many similar problems.

To get a flavour for the technique, which is described in detail in Appendix G, let's discover the first two solutions by trying the very simple form:

$$H(\xi) = A_n \xi^n. \tag{11}$$

To be a solution for $A_n \neq 0$ we have, on substituting into Hermite's equation,

$$n(n-1)\xi^{n-2} - 2n\xi^n + (\epsilon - 1)\xi^n = 0. \tag{12}$$

Since this must be true for all ξ, the coefficients of each separate power of ξ must vanish: for ξ^{n-2} we require $n(n-1) = 0$, giving two possibilities, $n = 0$ or $n = 1$; for the coefficient of ξ^n we require $\epsilon = 2n + 1$, or, $\epsilon = 1$ or $\epsilon = 2$. Using our definition of ϵ we therefore find the energy eigenvalues and the corresponding eigenstates, the ground state and first excited state wave functions:

$$\psi_0(x) = A_0 e^{-\frac{1}{2}\beta^2 x^2} \quad \text{with} \quad E_0 = \frac{1}{2}\hbar\omega_0 \tag{13}$$

$$\psi_1(x) = A_1 x e^{-\frac{1}{2}\beta^2 x^2} \quad \text{with} \quad E_1 = \frac{3}{2}\hbar\omega_0 \tag{14}$$

(I have incorporated some constant factors into A_1.) From the pattern of these solutions we may *guess* that the higher states correspond to higher powers of ξ, and that the n-th eigenstate ψ_n is an n-th order polynomial in x with eigenvalue

$$\begin{aligned} \epsilon &= (2n+1), \qquad n = 0, 1, 2, \ldots \\ \text{i.e.} \quad E_n &= \hbar\omega_0 \left(n + \frac{1}{2}\right) \end{aligned} \tag{15}$$

Note too that the parities are definite and alternate: even parity for even n; odd for odd n; that the energy eigenstates are also parity eigenstates follows from the symmetry of the oscillator potential under $x \to -x$.

We will not pursue the elementary but rather tedious solution by series here; instead we will find all the solutions by a wonderfully elegant and simple operator technique. This is not only interesting in its own right and as a method for finding the general solution to this particular problem, but it is also good practice in operator manipulation; but its usefulness goes well beyond this problem: these operators are examples of creation and annihilation operators used in relativistic quantum field theory to represent the creation and annihilation of elementary particles (such as the photon) allowed by Einstein's energy-mass equivalence, $E = mc^2$.

SOLVING THE HARMONIC OSCILLATOR USING OPERATORS.

This alternative elegant way of solving the quantum harmonic oscillator makes use of a non-Hermitian operator $\widehat{a}$ and its Hermitian conjugate $\widehat{a}^\dagger$. These operators have a wider significance in quantum physics: they are examples of lowering and raising operators, similar to those we will encounter in the theory of angular momentum; in the development of relativistic quantum field theory in elementary particle physics, they are like the operators that create and destroy particles - in this case, photons; and they are used extensively in the expanding field of quantum optics.

The following considerations may help to motivate the introduction of the operator $\widehat{a}$. We begin with the Hamiltonian, which is quadratic in both the operators $\widehat{p}$ and $\widehat{x} \equiv x$. Suppose we try to exploit this symmetry fully by writing the Hamiltonian as a quadratic in *dimensionless* Hermitian operators $\widehat{\mathcal{P}}$ and $\widehat{\mathcal{Q}}$

$$\widehat{H} = \frac{1}{2}\left(\frac{\widehat{p}^2}{m} + m\omega_0^2 x^2\right) \tag{16}$$

$$= \frac{1}{2}\hbar\omega_0\left(\widehat{\mathcal{P}}^2 + \widehat{\mathcal{Q}}^2\right) \tag{17}$$

We can see immediately that

$$\widehat{\mathcal{P}} = \left(\frac{1}{\hbar m\omega_0}\right)^{\frac{1}{2}}\widehat{p} \tag{18}$$

$$\equiv \alpha\widehat{p} \tag{19}$$

$$\widehat{\mathcal{Q}} = \left(\frac{m\omega_0}{\hbar}\right)^{\frac{1}{2}}\widehat{x} \tag{20}$$

$$\equiv \beta\widehat{x} \tag{21}$$

where,

$$\alpha \equiv \left(\frac{1}{\hbar m\omega_0}\right)^{\frac{1}{2}} \quad \text{and} \quad \beta \equiv \left(\frac{m\omega_0}{\hbar}\right)^{\frac{1}{2}} \tag{22}$$

Also notice the very useful result used several times later,

$$\hbar\alpha\beta = 1 \tag{23}$$

From the canonical commutation relation $[\widehat{x}, \widehat{p}] = i\hbar$ and the fact that $\hbar\alpha\beta = 1$ we find that these new operators obey the commutation law,

$$[\widehat{\mathcal{Q}}, \widehat{\mathcal{P}}] = i \tag{24}$$

We now define new dimensionless, but not Hermitian, operators which turn out to have both remarkable and useful properties: [3]

$$\widehat{a} \equiv \frac{1}{\sqrt{2}}(\widehat{\mathcal{Q}} + i\widehat{\mathcal{P}}) \tag{27}$$

$$\widehat{a}^\dagger \equiv \frac{1}{\sqrt{2}}(\widehat{\mathcal{Q}} - i\widehat{\mathcal{P}}) \tag{28}$$

Notice that we can write our favourite Hermitian operators $\widehat{x}$ and $\widehat{p}$ as simple combinations:

$$\widehat{x} = \frac{1}{\sqrt{2}\beta}\left(\widehat{a} + \widehat{a}^\dagger\right) \quad \text{and} \quad \widehat{p} = \frac{-i}{\sqrt{2}\alpha}\left(\widehat{a} - \widehat{a}^\dagger\right) \tag{29}$$

[3]These operators are the lowering and raising operators for the SHO. The application of $\widehat{a}$ to an energy eigenstate moves it down one step in the energy-level diagram; $\widehat{a}^\dagger$ moves it up one step:

$$\widehat{a}\psi_n = \sqrt{n}\psi_{n-1} \tag{25}$$

$$\widehat{a}^\dagger\psi_n = \sqrt{n+1}\psi_{n+1} \tag{26}$$

These can also be proved by using the results obtained in (c) and (d) below: see also Appendix E.

We can also solve these for the operators $\widehat{a}$ and $\widehat{a}^\dagger$ in terms of $\widehat{x}$ and $\widehat{p}$:

$$\widehat{a} \equiv \frac{1}{\sqrt{2}}\left(\beta\widehat{x} + i\,\alpha\widehat{p}\right) \quad \text{and} \quad \widehat{a}^\dagger \equiv \frac{1}{\sqrt{2}}\left(\beta\widehat{x} - i\,\alpha\widehat{p}\right) \tag{30}$$

We now phrase our operator solution of the quantum harmonic oscillator as a series of statements followed by their proofs:

(a) The operators $\widehat{a}$ and $\widehat{a}^\dagger$ obey the very simple commutation relation:

$$[\widehat{a}, \widehat{a}^\dagger] = 1 \tag{31}$$

(b) The harmonic oscillator Hamiltonian can be written in the form:

$$\widehat{H} = \hbar\omega_0\left(\widehat{a}^\dagger\widehat{a} + \frac{1}{2}\right) \tag{32}$$

(c) The lowering operator $\widehat{a}$ destroys the ground state eigenfunction:

$$\psi_0(x) = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} e^{-\beta^2x^2/2} \tag{33}$$

$$\widehat{a}\psi_0 = 0 \tag{34}$$

(d) Hence we can show that all eigenfunctions may be found by successive applications of the raising operator $\widehat{a}^\dagger$:

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\widehat{a}^{\dagger n}\psi_0(x), \tag{35}$$

i.e. $\psi_n(x)$ is an eigenfunction of $\widehat{H}$ corresponding to the energy $E_n = \hbar\omega_0(n + \frac{1}{2}),\ n = 0, 1, 2\ldots$

(e) Finally we check that the first two or three of these are indeed the solutions given in lectures.

Note: Only for parts (c) and (e) do we need to use the explicit representation $\widehat{p} = -i\hbar\partial/\partial x$; in all other cases we need only use the algebraic properties of the operators, all derived from the canonical commutator $[x, \widehat{p}] = i\hbar$.

Note that this is a *general* proof for the energy spectrum and eigenfunctions of the harmonic oscillator, with one proviso: I have not proved that ψ_0 is the ground state, but assumed that it is; the text book proofs are significantly longer because they actually prove that there is no state of lower energy than ψ_0.

THE PROOFS.

(a) The simplest way of evaluating the commutator is to find expressions for $\widehat{a}\,\widehat{a}^\dagger$ and $\widehat{a}^\dagger\widehat{a}$ in terms of the Hamiltonian:

$$\widehat{a}\,\widehat{a}^\dagger = \frac{1}{2}\left\{\widehat{\mathcal{Q}}^2 + \widehat{\mathcal{P}}^2 + i(\widehat{\mathcal{Q}}\widehat{\mathcal{P}} - \widehat{\mathcal{P}}\widehat{\mathcal{Q}}\right\} \tag{36}$$

$$= \frac{1}{2}\left\{\widehat{\mathcal{Q}}^2 + \widehat{\mathcal{P}}^2 - 1\right\} \tag{37}$$

where we used the commutation law for $\widehat{\mathcal{P}}$ and $\widehat{\mathcal{Q}}$. Recognising the Hamiltonian in the last line, we obtain our final expression:

$$\widehat{a}\,\widehat{a}^\dagger = \frac{1}{\hbar\omega_0}\widehat{H} + \frac{1}{2}, \tag{38}$$

$$\text{and similarly,} \quad \widehat{a}^\dagger\widehat{a} = \frac{1}{\hbar\omega_0}\widehat{H} - \frac{1}{2} \tag{39}$$

By subtracting these two expressions the Hamiltonian cancels out and we immediately obtain the commutator,

$$[\widehat{a}, \widehat{a}^\dagger] = 1 \tag{40}$$

In Appendix A we give a more direct, but longer, proof of this result.

(b) The required expression for the Hamiltonian is immediately found from the formula for $\widehat{a}^\dagger\widehat{a}$: [4]

$$\widehat{H} = \hbar\omega_0\left(\widehat{a}^\dagger\widehat{a} + \frac{1}{2}\right) \tag{41}$$

In Appendix B we give a more direct, but longer, proof of this result.

(c) Here we must use the explicit representation of the operators:

$$\widehat{p} = -i\hbar\frac{d}{dx}$$

$$\text{and therefore,} \quad \widehat{a} \equiv \frac{1}{\sqrt{2}}\left(\beta\widehat{x} + i\,\alpha\widehat{p}\right) = \frac{1}{\sqrt{2}}\left(\beta x + \hbar\alpha\frac{d}{dx}\right)$$

$$\begin{aligned}\text{Hence,} \quad \widehat{a}\psi_0(x) &= \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2}}\left(\beta x + \hbar\alpha\frac{d}{dx}\right)e^{-\frac{1}{2}\beta^2x^2} \\ &= \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2}}\left(\beta x - \hbar\alpha\beta^2 x\right)e^{-\frac{1}{2}\beta^2x^2} \\ &= 0 \qquad\qquad \text{QED.}\end{aligned}$$

where the 2nd term in brackets simplifies because $\hbar\alpha\beta = 1$ and therefore cancels the first term.

(d) To obtain the higher excited states we need the following useful results:

$$\left[\widehat{H}, \widehat{a}^\dagger\right] = \hbar\omega_0\widehat{a}^\dagger \tag{42}$$

$$\left[\widehat{H}, \widehat{a}\right] = -\hbar\omega_0\widehat{a} \tag{43}$$

Proof: In this proof we use the commutator

$$[\widehat{a}, \widehat{a}^\dagger] = 1$$

$$\text{in the form,} \quad \widehat{a}\,\widehat{a}^\dagger = \widehat{a}^\dagger\widehat{a} + 1 \tag{44}$$

[4] Although we can also express the Hamiltonian in terms of $\widehat{a}\,\widehat{a}^\dagger$, this is not as useful. The reason is that the operator $\widehat{a}$ destroys the ground state ψ_0 and therefore eliminates several terms by acting first.

to reorder the factors $\hat{a}^\dagger\hat{a}\hat{a}^\dagger$ into the form $\hat{a}^\dagger\hat{a}^\dagger\hat{a}$.

$$\begin{aligned}
[\hat{H},\hat{a}^\dagger] &= \hat{H}\hat{a}^\dagger - \hat{a}^\dagger\hat{H} \\
&= \hbar\omega_0\left\{(\hat{a}^\dagger\hat{a}+\frac{1}{2})\hat{a}^\dagger - \hat{a}^\dagger(\hat{a}^\dagger\hat{a}+\frac{1}{2})\right\} \qquad \text{using the formula in (b) for } \hat{H}; \\
&= \hbar\omega_0\left\{\hat{a}^\dagger(\hat{a}\hat{a}^\dagger) - \hat{a}^\dagger\hat{a}^\dagger\hat{a}\right\} \quad \text{with terms } \frac{1}{2}\hat{a}^\dagger \text{ cancelling;} \\
&= \hbar\omega_0\left\{\hat{a}^\dagger(\hat{a}^\dagger\hat{a}+1) - \hat{a}^\dagger\hat{a}^\dagger\hat{a}\right\} \\
&= \hbar\omega_0\hat{a}^\dagger \qquad \text{QED.}
\end{aligned} \tag{45}$$

The second commutator can be obtained by simply taking the dagger of both sides of the first and remembering that the commutator will change sign because the dagger operation changes the order of operators:

$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$$

We prove that $\psi_n \propto \hat{a}^{\dagger n}\psi_0$ is an energy eigenstate by induction: first we prove that for $n=0$, $\psi_{n=0} \equiv \psi_0$ is an eigenstate; then we prove that if ψ_n is one then so is ψ_{n+1}; hence ψ_n is an eigenstate for all $n = 0, 1, 2, \ldots$. [5]
For $n = 0$, it is obvious that ψ_0 is an eigenstate: since $\hat{a}$ annihilates the state (see (c)), the Hamiltonian in the form obtained in (b) gives,

$$\begin{aligned}
\hat{H}\psi_0 &= \hbar\omega_0(\hat{a}^\dagger\hat{a}+\frac{1}{2})\psi_0 \\
&= \frac{\hbar\omega_0}{2}\psi_0 \\
\text{i.e.} \qquad \hat{H}\psi_0 &= E_0\psi_0, \qquad \text{where } E_0 = \frac{\hbar\omega_0}{2} \text{ is the energy eigenvalue} \quad \text{QED.}
\end{aligned} \tag{46}$$

Now let us assume that ψ_n is an eigenstate:

$$\hat{H}\psi_n = E_n\psi_n \tag{47}$$

Operating on this state with $[\hat{H},\hat{a}^\dagger] = \hbar\omega_0\hat{a}^\dagger$,

$$\begin{aligned}
[\hat{H},\hat{a}^\dagger]\psi_n &= \hbar\omega_0(\hat{a}^\dagger\psi_n) \\
&= \hat{H}(\hat{a}^\dagger\psi_n) - \hat{a}^\dagger(\hat{H}\psi_n) \quad \text{expanding out the commutator;} \\
&= \hat{H}(\hat{a}^\dagger\psi_n) - E_n(\hat{a}^\dagger\psi_n) \quad \text{using} \quad \hat{H}\psi_n = E_n\psi_n; \\
\text{rearranging terms, we find} \quad \hat{H}(\hat{a}^\dagger\psi_n) &= (E_n + \hbar\omega_0)(\hat{a}^\dagger\psi_n)
\end{aligned} \tag{48}$$

which shows that [6]

$$\psi_{n+1} \propto \hat{a}^\dagger\psi_n \quad \text{is an eigenstate with energy eigenvaue} \quad E_n + \hbar\omega_0 \quad \text{QED.} \tag{49}$$

This completes the proof by induction, since now, starting from the $n = 0$ eigenstate ψ_0 with eigenvalue $E_0 = \hbar\omega_0/2$, we can construct the entire ladder of eigenstates by successive increments of n, ie. by operating successively with the ladder raising operator $\hat{a}^\dagger$.
To find the energy eigenvalue E_n is easy: each application of the raising operator increases the energy eigenvalue by $\hbar\omega_0$; to get the state ψ_n with energy E_n from the state ψ_0 with energy $E_0 = \hbar\omega_0/2$ requires the application of n raising operators, therefore increasing the energy eigenvalue by n units of $\hbar\omega_0$,

$$E_n = \hbar\omega_0(n+\frac{1}{2}), \quad n = 0, 1, 2, \ldots \qquad \text{QED.} \tag{50}$$

[5] Induction is simply a way to generalise the process of applying the operator $\hat{a}^{\dagger n}$ repeatedly, one at a time. See Appendix C for another proof by induction contrasted with the 'direct' proof.

[6] Notice that this result, equation (49), establishes that $\hat{a}^\dagger$ is the raising operator. In Appendix E we show that $\hat{a}$ is the lowering operator and discuss the normalisation of ψ_n with the factor $1/\sqrt{n!}$.

In Appendix D we give another proof of this result, which is lengthy because it needs to use the commutator proved in Appendix C.

(e) Taking the expression for the n-th eigenstate,

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\hat{a}^{\dagger n}\psi_0(x) \qquad \text{where} \qquad \psi_0(x) = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\beta^2 x^2}$$

Putting $n = 0$ and using $0! = 1$ immediately gives $\psi_{n=0} = \psi_0$, the ground state wave function as expected.

n=1:

$$\begin{aligned}
\psi_1(x) &= \frac{1}{\sqrt{1!}}\hat{a}^{\dagger}\psi_0(x) \\
&= \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2}}\left(\beta x - i\alpha(-i\hbar\frac{d}{dx})\right) e^{-\frac{1}{2}\beta^2 x^2} \qquad \text{using the given expression for } \hat{a}^{\dagger} \\
&= \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2}}\left(\beta x - \hbar\alpha\frac{d}{dx}\right) e^{-\frac{1}{2}\beta^2 x^2} \\
&= \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2}}\left(\beta x + \hbar\alpha\beta^2 x\right) e^{-\frac{1}{2}\beta^2 x^2} \qquad \text{Now using from part (a)} \ \ \hbar\alpha\beta = 1 \\
&= \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \sqrt{2}\beta x e^{-\frac{1}{2}\beta^2 x^2} \qquad \text{QED.}
\end{aligned}$$

The subsequent wave functions build on this since the general expression for ψ_n can be written as the action of $\hat{a}^{\dagger}$ on the previous ψ_{n-1}:

$$\begin{aligned}
\psi_n(x) &= \frac{1}{\sqrt{n!}}\hat{a}^{\dagger n}\psi_0(x) \\
&= \frac{1}{\sqrt{n}}\hat{a}^{\dagger}\left[\frac{1}{\sqrt{(n-1)!}}\hat{a}^{\dagger n-1}\psi_0(x)\right] \\
&= \frac{1}{\sqrt{n}}\hat{a}^{\dagger}\left[\psi_{n-1}(x)\right],
\end{aligned}$$

where, in the last step, we identified the quantity in the square brackets as ψ_{n-1}.
Applying this for $n = 2$ and using our previous expression for ψ_1,

n=2:

$$\begin{aligned}
\psi_2(x) &= \frac{1}{\sqrt{2}}\hat{a}^{\dagger}\left[\psi_1(x)\right] \\
&= \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}\left(\beta x - \hbar\alpha\frac{d}{dx}\right)\right]\left[\left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}}\sqrt{2}\beta x e^{-\frac{1}{2}\beta^2 x^2}\right] \\
&= \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2}}\beta(\beta x^2 - \hbar\alpha + \hbar\alpha\beta^2 x^2)e^{-\frac{1}{2}\beta^2 x^2}. \qquad \text{Now use from (a),} \ \ \hbar\alpha\beta = 1 \\
&= \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2}}(2\beta^2 x^2 - 1)e^{-\frac{1}{2}\beta^2 x^2} \qquad \text{QED.}
\end{aligned}$$

The general form of the normalised wave functions is:

$$\psi_n(x) = \left(\frac{\beta^2}{\pi}\right)^{\frac{1}{4}}\left(\frac{1}{2^n\, n!}\right)^{\frac{1}{2}} H_n(\beta\, x)e^{-\frac{1}{2}\beta^2 x^2}$$

where $H_n(\beta\, x)$ is the Hermite polynomial of order n.

$H_0(\xi) = 1$; $H_1(\xi) = 2\xi$; $H_2(\xi) = 4\xi^2 - 2$; $H_3(\xi) = 8\xi^3 - 12\xi$;
$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$; $H_5(\xi) = 32\xi^5 - 160\xi^3 + 120\xi$; $H_6(\xi) = 64\xi^6 - 480\xi^4 + 720\xi^2 - 120$;
$H_7(\xi) = 128\xi^7 - 1344\xi^5 + 3360\xi^3 - 1680\xi$; $H_8(\xi) = 256\xi^8 - 3584\xi^6 + 13440\xi^4 - 13440\xi^2 + 1680$.

APPENDIX A.

Note that $\widehat{a}^\dagger$ has the form it does because both $x = x^\dagger$ and $\widehat{p} = \widehat{p}^\dagger$ are Hermitian, while the dagger operation takes the complex conjugate of numbers such as $i\alpha$. Using our definitions,

$$\begin{aligned}
[\widehat{a}, \widehat{a}^\dagger] &= \frac{1}{2}\beta^2[\widehat{x}, \widehat{x}] + \frac{1}{2}\alpha^2[\widehat{p}, \widehat{p}] - \frac{1}{2}i\beta\alpha[\widehat{x}, \widehat{p}] + \frac{1}{2}i\alpha\beta[\widehat{p}, \widehat{x}] \\
&= 0 + 0 - i\beta\alpha[\widehat{x}, \widehat{p}] \\
&= (-i\beta\alpha)(i\hbar) \quad \text{using} \quad [\widehat{x}, \widehat{p}] = i\hbar \\
&= \hbar\beta\alpha = \hbar\left(\frac{m\omega_0}{\hbar}\frac{1}{\hbar m\omega_0}\right)^{\frac{1}{2}} \\
&= 1 \qquad \text{QED.}
\end{aligned}$$

APPENDIX B.

Using the definitions of $\widehat{a}$ and $\widehat{a}^\dagger$,

$$\begin{aligned}
\widehat{a}^\dagger\widehat{a} &= \frac{1}{2}(\beta\widehat{x} - i\alpha\widehat{p})(\beta\widehat{x} + i\alpha\widehat{p}) \\
&= \frac{1}{2}(\beta^2\widehat{x}^2 + \alpha^2\widehat{p}^2 + i\alpha\beta(\widehat{x}\widehat{p} - \widehat{p}\widehat{x}) \\
&= \frac{1}{2}\left(\alpha^2\widehat{p}^2 + \beta^2x^2 + i\alpha\beta(i\hbar)\right) \quad \text{using} \quad (\widehat{x}\widehat{p} - \widehat{p}\widehat{x}) = [\widehat{x}, \widehat{p}] = i\hbar \\
&= \frac{\widehat{p}^2}{2m}\frac{1}{\hbar\omega_0} + \frac{1}{2}m\omega_0^2x^2\frac{1}{\hbar\omega_0} - \frac{1}{2}.
\end{aligned}$$

Hence,

$$\begin{aligned}
\widehat{H} &= \frac{\widehat{p}^2}{2m} + \frac{1}{2}m\omega_0^2x^2 \\
&= \hbar\omega_0(\widehat{a}^\dagger\widehat{a} + \frac{1}{2}) \qquad \text{QED.}
\end{aligned}$$

APPENDIX C.

To get a general proof we first need to show that:

$$[\widehat{a}, \widehat{a}^{\dagger n}] = n\widehat{a}^{\dagger n-1} \tag{51}$$

I give you two methods: first the elegant proof by induction; second the sledge-hammer 'direct' proof by working it all out (which is really just induction in disguise!).
INDUCTION: The result is true for $n = 1$ because this has just been proved in part (a) above. Now assume the result is true for a given n; we will then show it to follow also for $(n + 1)$; it then follows that, starting from $n = 1$ (which we know to be true) we can deduce that it's true for all subsequent $n = 1 + 1 = 2, 2 + 1 = 3, \ldots$ and so on ad infinitum. This is proof by induction.
So, let us assume the truth, for some n, of

$$[\widehat{a}, \widehat{a}^{\dagger n}] = n\widehat{a}^{\dagger n-1}$$

Multiply this on the left by $\widehat{a}^\dagger$:

$$\begin{aligned}
\widehat{a}^\dagger[\widehat{a}, \widehat{a}^{\dagger n}] &= n\widehat{a}^{\dagger n} \\
&= \widehat{a}^\dagger\widehat{a}\,\widehat{a}^{\dagger n} - \widehat{a}^{\dagger n+1}\widehat{a} \\
&= (\widehat{a}\,\widehat{a}^\dagger - 1)\widehat{a}^{\dagger n} - \widehat{a}^{\dagger n+1}\widehat{a} \quad \text{using} \quad [\widehat{a}, \widehat{a}^\dagger] = 1 \\
&= [\widehat{a}, \widehat{a}^{\dagger n+1}] - \widehat{a}^{\dagger n}
\end{aligned}$$

Taking the last term to the other side (see the first line of the above equation) then gives

$$[\hat{a}, \hat{a}^{\dagger n+1}] = (n+1)\hat{a}^{\dagger n}.$$

This is just the starting assumption with n replaced by $n+1$: we have therefore shown that if it's true for a given n then it's true for the next one, $n+1$. Since it's true for $n=1$, it is therefore true for all n.QED.

DIRECT PROOF: We start with $[\hat{a}, \hat{a}^\dagger] = 1$ ie. $\hat{a}\,\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1$
Now apply this last equation repeatedly (n times) to $\hat{a}\,\hat{a}^{\dagger n}$ in order to interchange the daggered and undaggered operators:

$$\begin{aligned}
[\hat{a}, \hat{a}^{\dagger n}] &= \hat{a}\,\hat{a}^{\dagger n} - \hat{a}^{\dagger n}\hat{a} \\
&= (\hat{a}\,\hat{a}^\dagger)\hat{a}^{\dagger n-1} - \hat{a}^{\dagger n}\hat{a} \\
&= (\hat{a}^\dagger\hat{a} + 1)\hat{a}^{\dagger n-1} - \hat{a}^{\dagger n}\hat{a} \\
&= \hat{a}^\dagger(\hat{a}\,\hat{a}^\dagger)\hat{a}^{\dagger n-2} + \hat{a}^{\dagger n-1} - \hat{a}^{\dagger n}\hat{a} \\
&= \hat{a}^\dagger(\hat{a}^\dagger\hat{a} + 1)\hat{a}^{\dagger n-2} + \hat{a}^{\dagger n-1} - \hat{a}^{\dagger n}\hat{a} \\
&= \hat{a}^{\dagger 2}(\hat{a}\,\hat{a}^\dagger)\hat{a}^{\dagger n-3} + 2\hat{a}^{\dagger n-1} - \hat{a}^{\dagger n}\hat{a} \\
&\;\vdots \\
&= \hat{a}^{\dagger n}\hat{a} + n\hat{a}^{\dagger n-1} - \hat{a}^{\dagger n}\hat{a} \\
&= n\hat{a}^{\dagger n-1} \qquad\qquad \text{QED.}
\end{aligned}$$

APPENDIX D.

Using the expression for the Hamiltonian obtained in part (b),

$$\hat{H}\psi_n(x) = \frac{\hbar\omega_0}{\sqrt{n!}}\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)\hat{a}^{\dagger n}\psi_0(x)$$

$$\begin{aligned}
\text{But,} \qquad \hat{a}^\dagger\hat{a}\,\hat{a}^{\dagger n} &= \hat{a}^\dagger(\hat{a}\,\hat{a}^{\dagger n}) \\
&= \hat{a}^\dagger(\hat{a}^{\dagger n}\hat{a} + n\hat{a}^{\dagger n-1}) \quad \text{using the commutator in Appendix C,} \\
&= \hat{a}^{\dagger n+1}\hat{a} + n\hat{a}^{\dagger n}
\end{aligned}$$

Using this result and $\hat{a}\psi_0 = 0$ from (c) to drop the first term, we find:

$$\begin{aligned}
\hat{H}\psi_n(x) &= \frac{\hbar\omega_0}{\sqrt{n!}}\left(n + \frac{1}{2}\right)\hat{a}^{\dagger n}\psi_0(x) \\
&= \hbar\omega_0\left(n + \frac{1}{2}\right)\psi_n(x) \qquad\qquad \text{QED.} \\
&= E_n\,\psi_n(x) \quad \text{where we identify the eigenvalue as } E_n = \hbar\omega_0\left(n + \frac{1}{2}\right)
\end{aligned}$$

APPENDIX E.

The Raising Operator $\hat{a}^\dagger$.

In proof (d) we have already shown that $\hat{a}^\dagger$ is the ladder raising operator, equation (49), but have not yet determined the coefficient, N_{n+1}:

$$\psi_{n+1} = N_{n+1}\hat{a}^\dagger\psi_n, \qquad n = 0, 1, 2, \ldots \tag{52}$$

Since we must normalise the eigenstates, this coefficient must be chosen so that if ψ_n is normalised, then so also is ψ_{n+1}. The condition that ψ_{n+1} is normalised, given that ψ_n is normalised leads to the following:

$$\begin{aligned}
\int \psi_{n+1}^* \psi_{n+1}\, dx &= 1 \\
&= |N_{n+1}|^2 \int (\widehat{a}^\dagger \psi_n)^* (\widehat{a}^\dagger \psi_n)\, dx \\
&= |N_{n+1}|^2 \int \psi_n^* (\widehat{a}\,\widehat{a}^\dagger \psi_n)\, dx \qquad \text{using the definition of the Hermitian congugate;} \\
&= |N_{n+1}|^2 \int \psi_n^* \left\{ \frac{\widehat{H}}{\hbar\omega_0} + \frac{1}{2} \right\} \psi_n\, dx \qquad \text{using eq. (39),} \quad \widehat{a}\,\widehat{a}^\dagger = \frac{\widehat{H}}{\hbar\omega_0} + \frac{1}{2}; \\
&= |N_{n+1}|^2 \int \psi_n^* \left\{ \frac{\hbar\omega_0(n+1/2)}{\hbar\omega_0} + \frac{1}{2} \right\} \psi_n\, dx \qquad \text{using} \quad \widehat{H}\psi_n = \hbar\omega_0(n+\frac{1}{2})\psi_n; \\
&= |N_{n+1}|^2 (n+1) \int \psi_n^* \psi_n\, dx \\
&= |N_{n+1}|^2 (n+1) \qquad \text{since } \psi_n \text{ is assumed normalised.}
\end{aligned}$$

Hence, comparing the first and last lines of this sequence,

$$\begin{aligned}
|N_{n+1}|^2 (n+1) &= 1 \\
\text{whence,} \quad N_{n+1} &= \frac{1}{\sqrt{n+1}}, \qquad \text{on choosing the positive square root.}
\end{aligned}$$

thereby establishing that

$$\psi_{n+1} = \frac{1}{\sqrt{n+1}}\, \widehat{a}^\dagger \psi_n, \qquad n = 0, 1, 2, \ldots \tag{53}$$

Since ψ_0 given in (c) is normalised, this equation ensures that all the ψ_n are also normalised when found by successive application (n-times) of the ladder raising operator to ψ_0.

Normalisation of ψ_n.

We can now establish the normalisation factor given in (d), equation (35). Since $\psi_{n=0} \equiv \psi_0$ is normalised, it follows by applying equation (53) successively for $n = 0, 1, 2, \ldots$ we can build up the normalisation factor of $1/\sqrt{n!}$ in (d), equation (35) through the following sequence:

$$\begin{aligned}
n = 0, \qquad \psi_1 &= \frac{1}{\sqrt{1}} \widehat{a}^\dagger \psi_0, \\
n = 1, \qquad \psi_2 &= \frac{1}{\sqrt{2}} \widehat{a}^\dagger \psi_1 \\
&= \frac{1}{\sqrt{1.2}} \widehat{a}^{\dagger 2} \psi_0, \\
n = 2, \qquad \psi_3 &= \frac{1}{\sqrt{3}} \widehat{a}^\dagger \psi_2 \\
&= \frac{1}{\sqrt{1.2.3}} \widehat{a}^{\dagger 3} \psi_0, \\
&\vdots \\
n \to n-1 \qquad \psi_n &= \frac{1}{\sqrt{n}} \widehat{a}^\dagger \psi_{n-1} \\
&= \frac{1}{\sqrt{1.2.3\ldots n}} \widehat{a}^{\dagger n} \psi_0, \\
\text{i.e.} \qquad \psi_n &= \frac{1}{\sqrt{n!}} \widehat{a}^{n\dagger} \psi_0 \qquad \text{is normalised,} \qquad \text{Q.E.D.}
\end{aligned}$$

The Lowering Operator $\widehat{a}$.

The proof that $\widehat{a}$ is the ladder lowering operator is a simple application of equation (38) and the raising operator equation (53) with $n \to n-1$:

$$
\begin{aligned}
\widehat{a}\psi_n &= \frac{1}{\sqrt{n}}\widehat{a}\,\widehat{a}^\dagger\psi_{n-1} \qquad \text{using eq. (53)} \quad \psi_n = \frac{1}{\sqrt{n}}\widehat{a}^\dagger\psi_{n-1}; \\
&= \frac{1}{\sqrt{n}}\left(\frac{\widehat{H}}{\hbar\omega_0}+\frac{1}{2}\right)\psi_{n-1} \qquad \text{using equation (38) for } \widehat{a}\,\widehat{a}^\dagger; \\
&= \frac{1}{\sqrt{n}}\left(\frac{\hbar\omega_0(n-1/2)}{\hbar\omega_0}+\frac{1}{2}\right)\psi_{n-1} \qquad \text{since } \psi_{n-1} \text{ is an eigenstate:} \quad \widehat{H}\psi_{n-1} = \hbar\omega_0(n-\frac{1}{2})\psi_{n-1}; \\
&= \frac{n}{\sqrt{n}}\psi_{n-1} \\
&= \sqrt{n}\psi_{n-1} \\
\text{i.e.} \quad \widehat{a}\psi_n &= \sqrt{n}\psi_{n-1} \qquad \text{Q.E.D.}
\end{aligned}
\tag{54}
$$

APPENDIX F.

Asymptotic form of the SHO wave function.

To simplify the dimensionless form of the SHO TISE,

$$\frac{d^2\psi}{d\xi^2} + (\epsilon - \xi^2)\psi = 0. \tag{55}$$

we first examine the large ξ (i.e. large x) behaviour of the wave function. This is accomplished by noticing that for large ξ the ϵ term can be neglected compared with the ξ^2 term:

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi, \qquad \text{for large enough } \xi. \tag{56}$$

We guess the solution by seeking a function which, when differentiated twice, yields a factor ξ^2 times itself; this is an exponential, not in ξ, but in ξ^2:

$$\psi \approx e^{\pm\frac{1}{2}\xi^2}, \qquad \text{for large } \xi. \tag{57}$$

Since the plus sign would give an unphysical wave function not vanishing at infinity, we can discard that guess. Now let's check our guess by differentiating it twice:

$$
\begin{aligned}
\frac{d^2}{d\xi^2}e^{-\frac{1}{2}\xi^2} &= \frac{d}{d\xi}\left(-\xi e^{-\frac{1}{2}\xi^2}\right) \\
&= (\xi^2-1)e^{-\frac{1}{2}\xi^2} \\
&\approx \xi^2 e^{-\frac{1}{2}\xi^2}, \qquad \text{dropping the -1 term which is} << \xi^2 \text{ for large } \xi,
\end{aligned}
$$

showing that our guess is indeed a large ξ solution. This is why it was convenient to write the wave function as

$$
\begin{aligned}
\psi(x) &= H(\xi)e^{-\frac{1}{2}\xi^2} \\
&= H(\beta x)e^{-\frac{1}{2}\beta^2x^2},
\end{aligned}
\tag{58}
$$

with the Gaussian carrying the dominant asymptotic behaviour of the wave function.

Asymptotic form for the solution to the Hermite equation.

In Appendix G we shall show how to search sytematically for the physically acceptable solutions to the Hermite equation,

$$\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (\epsilon - 1)H = 0. \tag{59}$$

Here we wish to show how a similar guessing procedure to the above can reveal the unphysical solution encountered in Appendix G as an infinite power series. This series, although convergent, has uacceptable asymptotic behaviour. In searching for the asymptotic behavior of the Hermite function $H(\xi)$, we first note that no term can yet be dropped compared to the others. Following our previous guess, let us try to find an exponential solution of the form,

$$H(\xi) \approx e^{a\xi^2}, \quad \text{for large} \quad \xi. \tag{60}$$

where we do not yet have any idea what value or sign the constant a might have. Now let's check our guess by differentiating it:

$$\begin{aligned} \frac{d}{d\xi}e^{a\xi^2} &= 2a\xi\, e^{a\xi^2} \\ \text{and,} \qquad \frac{d^2}{d\xi^2}e^{a\xi^2} &= 2a\,\frac{d}{d\xi}\left(\xi\, e^{a\xi^2}\right) \\ &= 2a(2a\xi^2+1)\,e^{a\xi^2} \\ &\approx 4a^2\xi^2 e^{a\xi^2}, \quad \text{dropping the } +1 \text{ term which is} << 2a\xi^2 \text{ for large } \xi. \end{aligned}$$

Substituting into the Hermite equation, we see that for our guess to be a solution we require,

$$\begin{aligned} 4a^2\xi^2e^{a\xi^2} - 4a\xi^2e^{a\xi^2} + (\epsilon-1)e^{a\xi^2} &= 0 \\ 4a(a-1)\xi^2e^{a\xi^2} &\approx 0 \quad \text{dropping the } (\epsilon-1) \text{ term for large } \xi. \end{aligned}$$

The only possibility is therefore $a = 1$, demonstrating that at least one asymptotic solution is: [7]

$$H(\xi) \approx e^{\xi^2}, \quad \text{for large} \quad \xi. \tag{61}$$

Note that this solution is not physically admissible: the wave function would not vanish at infinity:

$$\begin{aligned} \psi(x) &= H(\xi)e^{-\frac{1}{2}\xi^2} \\ &\approx e^{\xi^2}e^{-\frac{1}{2}\xi^2}, \quad \text{for large } \xi \\ &\approx e^{+\frac{1}{2}\xi^2}, \quad \text{for large } \xi \end{aligned} \tag{62}$$

It would therefore seem that no solution can be found with acceptable asymptotic behaviour; but in fact we have not discovered all the possible solutions to Hermite's equation. In Appendix G we show that there is a way out through a clever choice for the energy term ϵ: the energy is quantised. If we choose $\epsilon = 2n + 1$ to be any odd integer, Hermite's equation has a polynomial solution of degree n leading to good asymptotic behaviour for the wave function:

$$\begin{aligned} \psi(x) &= H(\xi)e^{-\frac{1}{2}\xi^2} \\ &\approx \xi^n\, e^{-\frac{1}{2}\xi^2}, \quad \text{for large } \xi \\ &\to 0 \quad \text{as} \quad \xi \to \infty \end{aligned} \tag{63}$$

Notice that the Taylor expansion of this asymptotic solution to Hermite's equation is obtained trivially from the Taylor expansion of e^y by identifying y as ξ^2:

$$e^y = 1 + y + \frac{y^2}{2!} + \frac{y^3}{3!} + \ldots \tag{64}$$

[7] We could have anticipated this result, because we had already noted that the other asymptotic solution to the TISE is

$$\psi \approx e^{+\frac{1}{2}\xi^2}$$

$$
\begin{aligned}
&= \sum_{n=0}^{\infty} \frac{1}{n!} y^n \qquad \text{with summation over } n = 0,1,2,3,\dots \\
&= \sum_{n=0}^{\infty} \frac{1}{n!} \xi^{2n} \qquad \text{with } y \equiv \xi^2 \\
&= \sum_{m=0}^{\infty} \frac{1}{(\frac{1}{2}m)!} \xi^m \qquad \text{with summation now over } m = 0,2,4,\dots
\end{aligned} \tag{65}
$$

Notice particularly that $m = 2n$ runs over the even numbers only, $m = 0, 2, 4, \dots$. The ratio of successive terms c_m and c_{m+2} in this series is:

$$
\begin{aligned}
\frac{c_{m+2}}{c_m} &= \frac{\xi^{m+2}}{\left(\frac{1}{2}\{m+2\}\right)!} \frac{(\frac{1}{2}m)!}{\xi^m} \\
&= \frac{1.2.3\dots(\frac{1}{2}m)\left(\frac{1}{2}\{m+2\}\right)}{1.2.3\dots(\frac{1}{2}m)} \xi^2 \\
&= \frac{2}{m} \xi^2
\end{aligned} \tag{66}
$$

This series and this ratio will play a crucial role in finding the series solution in Appendix G.

APPENDIX G.

Solution by Series: the Fredholm method.

Here we show how Hermite's equation can be solved by a systematic method developed by Fredholm. We use the fact that almost any function can be written as a power series - the Taylor or the Maclaurin series - to make a guess at the solution which should be able to find all functions satisfying the differential equation. In fact Fredholm's method is a little more general: by introducing an extra parameter k it even allows negative or non-integral powers. We therefore search for solutions which can be written as a series:

$$H(\xi) = \sum_{n=0}^{\infty} a_n \, \xi^{n+k} \tag{67}$$

where both k and the infinitely many constants a_n are to be determined by demanding that this series be a solution to Hermite's equation. We first work out the derivatives:

$$H' = \sum_{n=0}^{\infty} a_n(n+k)\, \xi^{n+k-1} \tag{68}$$

Therefore the first derivative term in Hermite's equation, $\xi H'$, is

$$\xi H' = \sum_{n=0}^{\infty} a_n(n+k)\, \xi^{n+k} \tag{69}$$

$$
\begin{aligned}
H'' &= \sum_{n=0}^{\infty} a_n(n+k)(n+k-1)\, \xi^{n+k-2} \\
&= a_0(k-1)k\, \xi^{k-2} + a_1 k(k+1)\, \xi^{k-1} + \sum_{m=0}^{\infty} a_{m+2}(m+k+1)(m+k+2)\, \xi^{m+k}
\end{aligned} \tag{70}
$$

In the second step we have written out the first two terms of the series ($n = 0$ and $n = 1$) explicitly because the powers $k-1$ and $k-2$ do not occur anywhere else; then we have renamed the summation variable as $m \equiv n-2$, i.e. we make the replacement $n = m+2$ in the series which runs from $n = 2 \to \infty$: the result is that the summation over the new variable m now runs from $m = 0 \to \infty$. Having done all this we can rename the summation variable in the series for H' as m instead of n. We can then combine the two series for H' and H'' when we substitute into the Hermite equation. The condition for our series to be a solution is therefore:

$$\begin{aligned} & a_0(k-1)k\,\xi^{k-2} + a_1 k(k+1)\,\xi^{k-1} \\ + \sum_{m=0}^{\infty} \left\{a_{m+2}(m+k+1)(m+k+2) - a_m\left[2(m+k)+1-\epsilon\right]\right\}\xi^{m+k} &= 0 \qquad (71) \end{aligned}$$

Now comes the clever step: this equation must hold for all values of the variable ξ, and since *different* powers of ξ are *independent* functions, therefore the coefficient of each different power of ξ vanishes:

$$\text{for } \xi^{k-2}: \quad a_0\,k(k-1) = 0 \qquad (72)$$

$$\text{for } \xi^{k-1}: \quad a_1\,k(k+1) = 0 \qquad (73)$$

$$\text{for } \xi^{m+k}: \quad a_{m+2} = \frac{2(m+k)+1-\epsilon}{(m+k+1)(m+k+2)} \quad \text{with } m = 0,1,2,\ldots \qquad (74)$$

First let us concentrate on the first two equations; there are 3 distinct ways to satisfy these:
(1) $k = 1$, with $a_0 \neq 0$ and $a_1 = 0$;
(2) $k = -1$, with $a_0 = 0$ and $a_1 \neq 0$;
(3) $k = 0$, with both $a_0 \neq 0$ and $a_1 \neq 0$.
If we choose the first option we would only discover half the solutions: those with even parity. The other half would then be found by using the second option. This would then yield all the independent solutions. By choosing the third option we can find all the solutions in one go. Putting $k = 0$ in the recurrence relation, equation (74), we obtain expressions for all the coefficients with even-numbered subscripts in terms of a_0; all the odd-numbered subscripts in terms of a_1:

$$a_{m+2} = \frac{(2m+1)-\epsilon}{(m+1)(m+2)}\,a_m \quad \text{with } m = 0,1,2,\ldots \qquad (75)$$

Thus, for $m = 0,2,4,\ldots$ we obtain the following sequence:

$$a_2 = \frac{(1-\epsilon)}{1.2}\,a_0 \quad \text{for } m = 0, \qquad (76)$$

$$\begin{aligned} a_4 &= \frac{(5-\epsilon)}{3.4}\,a_2 \quad \text{for } m = 2, \\ &= \frac{(1-\epsilon)(5-\epsilon)}{1.2.3.4}\,a_0 \quad \text{where we used the } m = 0 \text{ step to replace } a_2; \qquad (77) \end{aligned}$$

$$\begin{aligned} a_6 &= \frac{(1-\epsilon)}{5.6}\,a_4 \quad \text{for } m = 4, \\ &= \frac{(1-\epsilon)(5-\epsilon)(9-\epsilon)}{1.2.3.4.5.6}\,a_0 \quad \text{where we used the } m = 2 \text{ step to replace } a_4; \qquad (78) \\ &\vdots \quad \textit{etc.} \end{aligned}$$

Displaying these steps explicitly shows:
(a) that *all* coefficients with even-numbered subscripts are expressible in terms of a_0, but
(b) that this sequence goes on for ever, *unless* one of the factors in the numerator, $(2m+1)-\epsilon = 0$; clearly this can happen *only* if ϵ is an odd-numbered integer.
For the odd integers, $m = 1,3,5,\ldots$ we obtain a similar sequence, but this time with the coefficients expressible in terms of a_1:

$$a_3 = \frac{(3-\epsilon)}{2.3}\,a_1 \quad \text{for } m = 1, \qquad (79)$$

$$\begin{aligned} a_5 &= \frac{(7-\epsilon)}{4.5}\,a_3 \quad \text{for } m = 3, \\ &= \frac{(3-\epsilon)(7-\epsilon)}{1.2.3.4.5}\,a_1 \quad \text{where we used the } m = 1 \text{ step to replace } a_3; \qquad (80) \end{aligned}$$

$$\begin{aligned} a_7 &= \frac{(11-\epsilon)}{6.7} a_5 \quad \text{for } m = 5, \\ &= \frac{(3-\epsilon)(7-\epsilon)(11-\epsilon)}{1.2.3.4.5.6.7} a_1 \quad \text{where we used the } m = 3 \text{ step to replace } a_5; \qquad (81) \\ &\vdots \quad etc. \end{aligned}$$

Displaying these steps explicitly shows:
(a) that ***all*** coefficients with odd-numbered subscripts are expressible in terms of a_1, but
(b) that this sequence goes on for ever, ***unless*** one of the factors in the numerator, $(2m+1) - \epsilon = 0$; clearly this can happen ***only*** if ϵ is an odd-numbered integer.

So far so good, but we now have to examine whether the two infinite series we have discovered give admissible wave functions. First we look at the convergence of the series by doing the ratio test for each of the two series, with even and odd powers of ξ respectively; thus successive terms in each series are $a_m \xi^m$ and $a_{m+2}\xi^{m+2}$:

$$\begin{aligned} \lim_{m\to\infty} \frac{a_{m+2}\xi^{m+2}}{a_m \xi^m} &= \lim_{m\to\infty} \frac{(m+1)(m+2)}{(2m+1)-\epsilon} \xi^2 \\ &= \lim_{m\to\infty} \frac{m}{2} \xi^2 \quad \text{since } m >> \text{ all the constants we dropped;} \qquad (82) \\ &= 0 \qquad (83) \end{aligned}$$

This is encouraging: both series converge for all values of ξ; but there is a problem with the asymptotic behaviour of both infinite series. We can see this by noticing that the ratio of successive terms in the series, equation (82), is the same as that for the Taylor expansion of e^{ξ^2}, equation (66). Thus the series of even powers of ξ behaves like e^{ξ^2}; the series of odd powers of ξ like $\xi\, e^{\xi^2}$, which is even worse. The result is that the wave function behaves asymptotically at least as badly as $e^{+\xi^2/2}$, as we saw in Appendix G, equation (62).
The way to avoid this catastrophe should now be clear: if $\epsilon = 2n+1$ for some integer n, then all terms in one of the two series from $m = n+2$ onwards would vanish. The series would then be a polynomial of degree n with the highest power of ξ determining the now benign asymptotic behaviour of the Hermite polynomial,

$$\begin{aligned} H(\xi) &\approx a_n\, \xi^n \quad \text{for large } \xi, \qquad (84) \\ \text{so that} \quad \psi(\xi) &= H(\xi) e^{-\frac{1}{2}\xi^2} \\ &\approx a_n\, \xi^n e^{-\frac{1}{2}\xi^2}, \quad \text{for large } \xi \qquad (85) \\ &\to 0 \quad \text{as} \quad \xi \to \infty. \qquad (86) \end{aligned}$$

This good asymptotic behaviour will only apply to the even series for n even, so the odd infinite series must be discarded as unphysical; if n is odd, then the even series must be discarded. Notice how our parity theorem is obeyed here: the even series gives a parity +1 wave function - the energy eigenstate; the odd series a parity -1 eigenstate. This is required by the symmetry of the SHO potential, $V(x) = m\omega_0^2\, x^2 = V(-x)$.
Clearly, since n can have any integer value from $n = 0$ onwards, we also discover the quantised energy eigenvalues:

$$\begin{aligned} \epsilon_n &= 2n+1, \quad \text{for } \; n = 0, 1, 2, \ldots; \qquad (87) \\ E_n &= \frac{\hbar\omega_0}{2}(2n+1) \\ &= \hbar\omega_0 (n + \frac{1}{2}), \quad \text{for } \; n = 0, 1, 2, \ldots \qquad (88) \end{aligned}$$

To find the energy eigenfunctions we first write down the recurrence relation for $\epsilon = 2n+1$:

$$a_{m+2} = \frac{(2m+1)-(2n+1)}{(m+1)(m+2)} a_m, \qquad (89)$$

$$= \quad -2\frac{(n-m)}{(m+1)(m+2)}a_m, \quad \text{for } m < n \tag{90}$$

$$\text{with } m = 0, 2, 4, \ldots \quad \text{for } n \text{ an even integer;}$$

$$\text{with } m = 1, 3, 5, \ldots \quad \text{for } n \text{ an odd integer.}$$

Remember to keep the integer n fixed at some definite value. Although it is quite straightforward to use the recurrence relation to obtain a closed formula for the nonzero a_m, we shall instead just illustrate its use for the first few eigenstates.
(0) For $n = 0$, $\epsilon = 1$ and eq. (76) tells us that $a_2 = 0$, and so are all the subsequent coefficients. Discarding the odd series - which is equivalent to taking $a_1 = 0$ - we have a series with just one term:

$$H_0(\xi) = a_0$$

$$\psi_0(\xi) = a_0\, e^{-\frac{1}{2}\xi^2}$$

where a_0 is obtained by normalising the wave function.
(1)For $n = 1$, $\epsilon = 3$ and eq. (79) tells us that $a_3 = 0$, and so are all the subsequent coefficients. Discarding the even series - which is equivalent to taking $a_0 = 0$ - we have a series with just one term:

$$H_1(\xi) = a_1\xi$$

$$\psi_1(\xi) = a_1\, \xi e^{-\frac{1}{2}\xi^2}$$

where a_1 is obtained by normalising the wave function.
(2) For $n = 2$, $\epsilon = 5$; eq. (76) tells us that $a_2 = -2a_0$; eq. (77) tells us that $a_4 = 0$ and so are all the subsequent coefficients. Discarding the odd series - which is equivalent to taking $a_1 = 0$ - we now have a series with two terms:

$$H_2(\xi) = -a_0(2\xi^2 - 1)$$

$$\psi_2(\xi) = -a_0(2\xi^2 - 1)e^{-\frac{1}{2}\xi^2}$$

where a_0 is obtained by normalising this wave function. (3)For $n = 3$, $\epsilon = 7$; eq. (79) tells us that $a_3 = -\frac{2}{3}a_1$; eq. (80) tells us that $a_5 = 0$, and so are all the subsequent coefficients. Discarding the even series - which is equivalent to taking $a_0 = 0$ - we have a series with two terms:

$$H_3(\xi) = -\frac{a_1}{3}(2\xi^3 - 3\xi)$$

$$\psi_1(\xi) = -\frac{a_1}{3}(2\xi^3 - 3\xi)e^{-\frac{1}{2}\xi^2}$$

where a_1 is obtained by normalising the wave function. We recognise these wave functions as precisely those we found by the simpler and more elegant operator method.
