The Quantum Harmonic Oscillator — Solving for Energies and Wavefunctions (Step-by-Step)

Goal. Starting from the Hamiltonian, derive **(i)** the allowed energies E_n and **(ii)** the normalized stationary wavefunctions $\psi_n(x)$ for a 1D harmonic oscillator. Every algebraic step is shown; nothing important is skipped.

---

0) Problem data and what we're solving

- Particle of mass m in potential $V(x) = \frac{1}{2}kx^2$.
- Define the angular frequency $\omega = \sqrt{k/m}$ so that $V(x) = \frac{1}{2}m\omega^2 x^2$.
- **Hamiltonian operator** (write this first):

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2, \qquad [\hat{x}, \hat{p}] = i\hbar.$$

- **What to solve:** the time-independent Schrödinger equation (TISE)

$$\hat{H}\,\psi(x) = E\,\psi(x) \quad \Longleftrightarrow \quad -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2\,\psi = E\,\psi.$$

---

1) Non-dimensionalize (choose natural units to simplify)

Reason. Converting to a dimensionless coordinate makes the equation symmetric and easier to solve.

1. **Define a natural length**

$$x_0 \equiv \sqrt{\frac{\hbar}{m\omega}} \quad (\text{has dimensions of length}).$$

2. **Define the dimensionless coordinate** ξ :

$$\xi \equiv \frac{x}{x_0}. \qquad \Rightarrow \qquad \frac{\mathrm{d}}{\mathrm{d}x} = \frac{1}{x_0}\frac{\mathrm{d}}{\mathrm{d}\xi}, \quad \frac{\mathrm{d}^2}{\mathrm{d}x^2} = \frac{1}{x_0^2}\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}.$$

3. **Substitute into the TISE** (do it term by term):
4. Kinetic term: $-\frac{\hbar^2}{2m}\frac{1}{x_0^2}\,\psi''(\xi)$.
5. Potential term: $\frac{1}{2}m\omega^2\,x^2\psi = \frac{1}{2}m\omega^2\,x_0^2\,\xi^2\psi$.

Using $x_0^2 = \hbar/(m\omega)$:

$$-\frac{\hbar^2}{2m}\frac{1}{x_0^2} = -\frac{\hbar^2}{2m}\frac{m\omega}{\hbar} = -\frac{\hbar\omega}{2}, \qquad \frac{1}{2}m\omega^2 x_0^2 = \frac{1}{2}m\omega^2\frac{\hbar}{m\omega} = \frac{\hbar\omega}{2}.$$

So the entire equation becomes

$$-\frac{\hbar\omega}{2}\,\psi''(\xi) + \frac{\hbar\omega}{2}\,\xi^2\psi(\xi) = E\,\psi(\xi).$$

4. **Divide both sides by** $\hbar\omega/2$ and define a dimensionless energy parameter

$$\lambda \equiv \frac{2E}{\hbar\omega}.$$

We get the compact **dimensionless Schrödinger equation**

$$-\psi''(\xi) + \xi^2\psi(\xi) = \lambda\,\psi(\xi). \tag{1}$$

> **Checkpoint (units).** λ is dimensionless; good. The equation has no explicit $m, \hbar, \omega$ left—only λ remembers the energy scale.

---

2) Large-$|\xi|$ behavior suggests a Gaussian factor

Idea. For $|\xi| \gg 1$, the $\xi^2\psi$ term dominates. If we ignore ψ'' temporarily, a trial solution behaves like $\psi \sim e^{-\xi^2/2}$ (decays) or $e^{+\xi^2/2}$ (blows up). Normalizability forces the decaying Gaussian.

Therefore, set

$$\psi(\xi) = e^{-\xi^2/2}\,y(\xi). \tag{Ansatz}$$

We'll solve for the polynomial-like part $y(\xi)$.

Compute derivatives carefully (showing every step):

$$\psi' = e^{-\xi^2/2}\,(y' - \xi y), \qquad \psi'' = e^{-\xi^2/2}\,\big(y'' - 2\xi y' + (\xi^2 - 1)y\big).$$

(Substitute these into Eq. (1).)

Left side of (1):

$$-\psi'' + \xi^2\psi = -e^{-\xi^2/2}\big(y'' - 2\xi y' + (\xi^2-1)y\big) + \xi^2 e^{-\xi^2/2}y = e^{-\xi^2/2}\big(-y'' + 2\xi y' + y\big).$$

Thus Eq. (1) becomes

$$e^{-\xi^2/2}\big(-y'' + 2\xi y' + y\big) = \lambda\,e^{-\xi^2/2}y.$$

Cancel the common factor $e^{-\xi^2/2}$:

$$-y'' + 2\xi y' + y = \lambda y \quad\Longleftrightarrow\quad y'' - 2\xi y' + (\lambda - 1)y = 0. \tag{2}$$

This is **Hermite's differential equation**.

---

3) Power-series solution and the recurrence relation

We now solve Eq. (2) by a power series. Assume

$$y(\xi) = \sum_{k=0}^{\infty} a_k \xi^k.$$

Then

$$y' = \sum_{k=1}^{\infty} k a_k \xi^{k-1}, \qquad y'' = \sum_{k=2}^{\infty} k(k-1) a_k \xi^{k-2}.$$

Substitute into Eq. (2):

$$\sum_{k=2}^{\infty} k(k-1) a_k \xi^{k-2} - 2\xi \sum_{k=1}^{\infty} k a_k \xi^{k-1} + (\lambda - 1) \sum_{k=0}^{\infty} a_k \xi^k = 0.$$

Re-index the first sum (let $m = k - 2$, so $k = m + 2$) and rewrite all sums with power ξ^m :

$$\sum_{m=0}^{\infty} (m+2)(m+1) a_{m+2} \xi^m - 2 \sum_{m=0}^{\infty} m a_m \xi^m + (\lambda - 1) \sum_{m=0}^{\infty} a_m \xi^m = 0.$$

Group coefficients of ξ^m (each must vanish):

$$(m+2)(m+1) a_{m+2} + \big[-2m + (\lambda - 1) \big] a_m = 0.$$

Solve for a_{m+2} :

$$a_{m+2} = \frac{2m + 1 - \lambda}{(m+2)(m+1)} \, a_m. \qquad \text{(Recurrence)}$$

This upward recursion generates all higher coefficients from a_0 and a_1 .

> **Parity note.** Because the recurrence links $m \to m + 2$, even and odd powers never mix. Choosing $a_0 \ / \ 0, a_1 = 0$ gives an **even** solution; choosing $a_0 = 0, a_1 \ / \ 0$ gives an **odd** solution. This matches the even potential $V(x) = V(-x)$.

---

4) Why energies are quantized (polynomial termination)

For large m , the recurrence roughly gives $a_{m+2} \sim (2m/(m+2)(m+1)) a_m$, which does **not** make the series terminate. If the series does not terminate, the resulting $y(\xi)$ grows like $e^{+\xi^2}$, and then $\psi(\xi) = e^{-\xi^2/2} y(\xi)$ diverges as $e^{+\xi^2/2}$: **not normalizable**.

Resolution: Demand the series **terminate** after some finite order n . Termination happens exactly when the numerator in the recurrence becomes zero:

$$2n + 1 - \lambda = 0 \quad \Longrightarrow \quad \boxed{\lambda = 2n + 1} \qquad (n = 0, 1, 2, \ldots)$$

Using $\lambda = 2E/(\hbar\omega)$, this gives the **quantized energies**

$$\boxed{E_n = \hbar\omega\left(n + \tfrac{1}{2}\right), \quad n = 0, 1, 2, \ldots}$$

With $\lambda = 2n + 1$, the series truncates and $y(\xi)$ is a degree-n polynomial. Those polynomials are (up to a constant factor) the **Hermite polynomials** $H_n(\xi)$.

---

5) Build the first few polynomials explicitly (see it work)

Take the recurrence with $\lambda = 2n + 1$ and compute:

(a) Even solutions (set $a_0 \; / \; 0, a_1 = 0$)

- For $n = 0 : \lambda = 1$. Recurrence gives $a_2 = \frac{1-1}{2\cdot 1} a_0 = 0 \Rightarrow$ series stops immediately.
  $y_0(\xi) = a_0$, so up to normalization $H_0(\xi) = 1$.
- For $n = 2 : \lambda = 5$. Starting with a_0 :
  $a_2 = \frac{1-5}{2\cdot 1} a_0 = -2a_0$;
  $a_4 = \frac{5-5}{4\cdot 3} a_2 = 0 \Rightarrow$ stop.
  Up to an overall factor, $H_2(\xi) = 4\xi^2 - 2$.

(b) Odd solutions (set $a_0 = 0, a_1 \; / \; 0$) $=$

- For $n = 1 : \lambda = 3$.
  $a_3 = \frac{3-3}{3\cdot 2} a_1 = 0 \Rightarrow$ stop.
  Up to an overall factor, $H_1(\xi) = 2\xi$.
- For $n = 3 : \lambda = 7$.
  $a_3 = \frac{3-7}{3\cdot 2} a_1 = -\frac{2}{3} a_1$, then $a_5 = 0$ etc.
  Up to an overall factor, $H_3(\xi) = 8\xi^3 - 12\xi$.

(These match the standard Hermite polynomials.)

---

6) Assemble the (unnormalized) wavefunctions

Recall $\psi(\xi) = e^{-\xi^2/2} y(\xi)$. When the series terminates at order n , $y \propto H_n(\xi)$. Thus

$$\psi_n(\xi) \propto e^{-\xi^2/2}\, H_n(\xi), \qquad \xi = \frac{x}{x_0}.$$

Restore x :

$$\psi_n(x) \propto e^{-x^2/(2x_0^2)}\, H_n\left(\frac{x}{x_0}\right), \qquad x_0 = \sqrt{\frac{\hbar}{m\omega}}.$$

Parity is automatic: H_n is even (odd) for even (odd) n , so $\psi_n(-x) = (-1)^n \psi_n(x)$.

---

7) Normalize the wavefunctions (find the constant)

We want $\int_{-\infty}^{\infty} |\psi_n(x)|^2 \, \mathrm{d}x = 1$. Change to $\xi = x/x_0$, so $\mathrm{d}x = x_0 \, \mathrm{d}\xi$:

$$1 = |\mathcal{N}_n|^2 \int_{-\infty}^{\infty} e^{-x^2/x_0^2} \left| H_n\left(\tfrac{x}{x_0}\right) \right|^2 \mathrm{d}x = |\mathcal{N}_n|^2 \, x_0 \int_{-\infty}^{\infty} e^{-\xi^2} H_n^2(\xi) \, \mathrm{d}\xi.$$

A standard (and provable) Hermite identity is

$$\int_{-\infty}^{\infty} e^{-\xi^2} H_n(\xi) H_m(\xi) \, \mathrm{d}\xi = \sqrt{\pi} \, 2^n n! \, \delta_{nm}.$$

Setting $m = n$ gives

$$1 = |\mathcal{N}_n|^2 \, x_0 \, (\sqrt{\pi} \, 2^n n!) \quad \Rightarrow \quad \boxed{\mathcal{N}_n = \frac{1}{\sqrt{\sqrt{\pi} \, 2^n n! \, x_0}}}.$$

Therefore the **normalized stationary states** are

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \, \frac{1}{\pi^{1/4} \sqrt{x_0}} \, H_n\left(\frac{x}{x_0}\right) \exp\left(-\frac{x^2}{2x_0^2}\right), \quad n = 0, 1, 2, \ldots}$$

with **energies** $\boxed{E_n = \hbar\omega(n + \frac{1}{2})}$.

> **Sanity checks.**
> • $n = 0 : H_0 = 1$ gives a Gaussian ground state.
> • $\langle x \rangle = 0$ (odd integrand) and $\langle x^2 \rangle = (n + \frac{1}{2}) x_0^2$ (can be shown via ladder operators or direct integrals).
> • Level spacing is constant: $E_{n+1} - E_n = \hbar\omega$.

---

8) Full method recap (as a recipe)

1. **Write TISE** with $V = \frac{1}{2} m\omega^2 x^2$.
2. **Define** $x_0 = \sqrt{\hbar/(m\omega)}$ and $\xi = x/x_0$, reduce to $-\psi'' + \xi^2 \psi = \lambda \psi$.
3. **Extract Gaussian**: set $\psi = e^{-\xi^2/2} y$, obtain $y'' - 2\xi y' + (\lambda - 1) y = 0$.
4. **Series solve**: $a_{m+2} = \dfrac{2m + 1 - \lambda}{(m+2)(m+1)} a_m$.
5. **Normalizability ⇒ termination**: require $\lambda = 2n + 1 \Rightarrow E_n = \hbar\omega(n + \frac{1}{2})$.
6. **Identify** $y \propto H_n$, so $\psi_n \propto e^{-\xi^2/2} H_n$.
7. **Normalize** using $\int e^{-\xi^2} H_n^2 \, \mathrm{d}\xi = \sqrt{\pi} 2^n n!$ to get the final prefactor.

---

9) Optional: Ground state derived by minimization (quick cross-check)

Using only uncertainties, estimate the ground-state energy $E(\Delta x) = \dfrac{\hbar^2}{8m(\Delta x)^2} + \dfrac{1}{2}m\omega^2(\Delta x)^2$.
Minimize over Δx : set derivative to zero → $(\Delta x)^2 = \hbar/(2m\omega) = x_0^2/2$.
Plug back: $E_{\min} = \frac{1}{2}\hbar\omega$, which matches E_0 .

---

10) Worked examples (plug-and-play)

(i) $n = 0$
$E_0 = \frac{1}{2}\hbar\omega$.
$\psi_0(x) = \dfrac{1}{\pi^{1/4}\sqrt{x_0}}\, e^{-x^2/(2x_0^2)}$.

(ii) $n = 1$
$E_1 = \frac{3}{2}\hbar\omega$.
$\psi_1(x) = \dfrac{1}{\sqrt{2}\,\pi^{1/4}\sqrt{x_0}}\left(2\,\frac{x}{x_0}\right) e^{-x^2/(2x_0^2)} = \sqrt{\frac{2}{\pi^{1/2}\,x_0^3}}\,x\,e^{-x^2/(2x_0^2)}$.

(iii) $n = 2$
$E_2 = \frac{5}{2}\hbar\omega$.
$\psi_2(x) = \dfrac{1}{\sqrt{8}\,\pi^{1/4}\sqrt{x_0}}\left(4\xi^2 - 2\right) e^{-\xi^2/2}$ with $\xi = x/x_0$.

---

11) Frequently-made mistakes (and how to avoid them)

- **Forgetting the Gaussian factor.** The polynomial alone is not normalizable; always include $e^{-\xi^2/2}$.
- **Dropping the** $+\frac{1}{2}$ in E_n . Remember the zero-point energy.
- **Confusing** x_0 with the ground-state width: $(\Delta x)_0 = x_0/\sqrt{2}$.
- **Mixing parity.** Start with either a_0 or a_1 , not both, to keep even/odd solutions clean.

Final boxed results

$$\boxed{E_n = \hbar\omega\left(n + \tfrac{1}{2}\right), \quad n = 0, 1, 2, \ldots}$$

$$\boxed{\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\,\frac{1}{\pi^{1/4}\,\sqrt{x_0}}\,H_n\!\left(\frac{x}{x_0}\right)\, e^{-x^2/(2x_0^2)}, \quad x_0 = \sqrt{\frac{\hbar}{m\omega}}}$$

If you’d like, we can add a short appendix proving the Hermite orthogonality integral, or a second solution using **ladder operators** to cross-verify the spectrum and matrix elements.