I. HARMONIC OSCILLATOR

Stationary Schrödinger equation forharmonic oscillator reads

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

Make a change of variable $y=x\sqrt{\frac{m\omega}{\hbar}} \Leftrightarrow x=y\sqrt{\frac{\hbar}{m\omega}} \Rightarrow$

$$y=x\sqrt{\frac{m\omega}{\hbar}} \quad\Leftrightarrow\quad x=y\sqrt{\frac{\hbar}{m\omega}} \quad\Rightarrow\quad \frac{d}{dx}\psi(x) \;=\; \sqrt{\frac{m\omega}{\hbar}}\frac{d}{dy}\psi(y) \tag{2}$$

and the Schrödinger Eq.(1) takes the form

$$\frac{d^2\psi(y)}{dy^2}-y^2\psi(y) \;=\; -2\mathcal{E}\psi(y) \tag{3}$$

where $\mathcal{E}\equiv\frac{E}{\hbar\omega}$ and the boundary conditions are as usual: $\psi(y)\to 0$ as $y\to\pm\infty$.

Useful rewriting: for any $f(y)$ write down formulas

$$\begin{aligned}(\frac{d}{dy}-y)(\frac{d}{dy}+y)f(y) &= \frac{d^2f(y)}{dy^2}-y^2f(y)+f(y)\\ (\frac{d}{dy}+y)(\frac{d}{dy}-y)f(y) &= \frac{d^2f(y)}{dy^2}-y^2f(y)-f(y)\end{aligned} \tag{4}$$

and rewrite them as follows

$$\begin{aligned}\tfrac{1}{2}(\tfrac{d}{dy}-y)(\tfrac{d}{dy}+y)f(y)+\tfrac{1}{2}(\tfrac{d}{dy}+y)(\tfrac{d}{dy}-y)f(y) &= \tfrac{d^2f(y)}{dy^2}-y^2f(y)\\ \tfrac{1}{2}(\tfrac{d}{dy}-y)(\tfrac{d}{dy}+y)f(y)-\tfrac{1}{2}(\tfrac{d}{dy}+y)(\tfrac{d}{dy}-y)f(y) &= f(y)\end{aligned} \tag{5}$$

First, let us prove that for any solution of Eq. (3) $\mathcal{E}$ is non-negative. Consider

$$\begin{aligned}&\int dy\ \psi^*(y)(\frac{d^2\psi(y)}{dy^2}-y^2\psi(y)) \\ &= \frac{1}{2}\int dy\ \psi^*(y)(\frac{d}{dy}-y)(\frac{d}{dy}+y)\psi(y)+\frac{1}{2}\int dy\ \psi^*(y)(\frac{d}{dy}+y)(\frac{d}{dy}-y)\psi(y)\\ &= -\frac{1}{2}\int dy\ \{(\frac{d}{dy}+y)\psi(y)\}^*(\frac{d}{dy}+y)\psi(y)-\frac{1}{2}\int dy\ \{(\frac{d}{dy}-y)\psi(y)\}^*(\frac{d}{dy}-y)\psi(y)\ \leq\ 0\end{aligned} \tag{6}$$

where we used first line in Eq. (8) and integration by parts. Thus, for any ψ the l.h.s. of Eq. (8) is negative which means that if ψ is a solution of Eq. (3)

$$\int dy\ \psi^*(y)(\frac{d^2\psi(y)}{dy^2}-y^2)\psi(y) \;=\; -2\mathcal{E}\int dy\ \psi^*(y)\psi(y) \;=\; -2\mathcal{E}\ \leq\ 0 \tag{7}$$

so $\mathcal{E}\geq 0$ in accordance with the classical picture.

Now, theorem:

If $f_n(y)$ is a solution of

$$\frac{d^2 f_n(y)}{dy^2} - y^2 f_n(y) \;=\; -2\mathcal{E}_n f_n(y) \tag{8}$$

the function

$$f_{n+1}(y) \;=\; (\frac{d}{dy} - y) f_n(y) \tag{9}$$

is a solution of the same equation with $\mathcal{E}_{n+1} = \mathcal{E}_n + 1$

$$\frac{d^2 f_{n+1}(y)}{dy^2} - y^2 f_{n+1}(y) \;=\; -2(\mathcal{E}+1) f_{n+1}(y) \tag{10}$$

Proof: first, we can rewrite $\frac{d^2\phi(y)}{dy^2} - y^2\phi(y)$ as follows

$$\frac{d^2\phi(y)}{dy^2} - y^2\phi(y) \;=\; (\frac{d}{dy} - y)(\frac{d}{dy} + y)\phi(y) - \phi(y) \;=\; (\frac{d}{dy} + y)(\frac{d}{dy} - y)\phi(y) + \phi(y) \tag{11}$$

Now, let us apply the formula (11) to $\phi(y) = f_{n+1}(y) = (\frac{d}{dy} - y) f_n(y)$

$$\begin{aligned} \frac{d^2 f_{n+1}(y)}{dy^2} - y^2 f_{n+1}(y) \;&=\; (\frac{d}{dy} - y)(\frac{d}{dy} + y) f_{n+1}(y) - f_{n+1}(y) \\ =\; &(\frac{d}{dy} - y)(\frac{d}{dy} + y)(\frac{d}{dy} - y) f_n(y) - (\frac{d}{dy} - y) f_n(y) \\ =\; &(\frac{d}{dy} - y)(-2\mathcal{E}_n - 1) f_n(y) - (\frac{d}{dy} - y) f_n(y) \;=\; (-2\mathcal{E}_n - 2)(\frac{d}{dy} - y) f_n(y) \\ =\; &-2(\mathcal{E}_n + 1) f_{n+1}(y), \qquad \text{Q.E.D.} \end{aligned} \tag{12}$$

Similarly, one can prove that

$$f_{n-1}(y) \;=\; (\frac{d}{dy} + y) f_n(y)$$

is a solution of the equation

$$\frac{d^2 f_{n-1}(y)}{dy^2} - y^2 f_{n-1}(y) \;=\; -2\mathcal{E}_{n-1} f_n(y) \tag{13}$$

with $\mathcal{E}_{n-1} = \mathcal{E}_n - 1$.

Now, assume that $\psi_n(y)$ is a solution of Eq. (3) with $\mathcal{E} = \mathcal{E}_n$. From eq. (13) we see that if we consider $(\frac{d}{dy} + y)^N \psi_n(y)$, we get a solution of Eq. (3) with $\mathcal{E} = \mathcal{E}_n - N$. Since for any solution $\mathcal{E} \geq 0$ this must stop at some N and the only way to stop is to get 0 at some step. Thus, the solution $\psi_0(y)$ with the lowest $\mathcal{E}$ must satisfy

$$(\frac{d}{dy} + y)\psi_0(y) \;=\; 0 \tag{14}$$

which easily yields

$$\psi_0(y) \;=\; e^{-\frac{y^2}{2}} \tag{15}$$

and

$$\mathcal{E}_0 \;=\; \frac{1}{2} \tag{16}$$

Next, from Eq. (10) we see that the solutions with $E_n = \frac{1}{2} + n$ can be obtained as

$$\psi_n(y) \;=\; \Big(\frac{d}{dy} - y\Big)^n e^{-\frac{y^2}{2}} \tag{17}$$

Now, let us return to the original variable $x = y\sqrt{\frac{\hbar}{m\omega}}$ and see what we have learned.

The wave function of the ground state is

$$\psi_0(x) \;=\; \Big(\frac{m\omega}{\pi\hbar}\Big)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2} \tag{18}$$

where the constant in front of the exponent was obtained from the normalization condition

$$\int dy |\psi_0(x)|^2 \;=\; \sqrt{\frac{m\omega}{\pi\hbar}}\int dx\; e^{-\frac{m\omega}{\hbar}x^2} \;=\; 1 \tag{19}$$

The energy of the ground state is

$$E_0 \;=\; \frac{\hbar\omega}{2} \tag{20}$$

The wave functions of excited states are obtained from Eq. (17)

$$\psi_0(x) \;=\; \Big(\sqrt{\frac{\hbar}{m\omega}}\frac{d}{dx} - x\sqrt{\frac{m\omega}{\hbar}}\Big)^n \Big(\frac{m\omega}{\pi\hbar}\Big)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2} \tag{21}$$

by proper normalization. The energies of the excited states are

$$E_n \;=\; \hbar\omega(\frac{1}{2} + n) \tag{22}$$

First few wave functons

$$\begin{aligned}
\psi_0(x) \;&=\; \Big(\frac{m\omega}{\pi\hbar}\Big)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}, \qquad \psi_1(x) \;=\; 2\sqrt{\frac{m\omega}{\hbar}}\Big(\frac{m\omega}{\pi\hbar}\Big)^{\frac{1}{4}} x e^{-\frac{m\omega}{2\hbar}x^2} \\
\psi_2(x) \;&=\; \frac{1}{\sqrt{2}}\Big(2\frac{m\omega}{\hbar}x^2 - 1\Big)\Big(\frac{m\omega}{\pi\hbar}\Big)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2} \\
\psi_3(x) \;&=\; \sqrt{\frac{m\omega}{3\pi\hbar}}\Big(2\frac{m\omega}{\hbar}x^3 - 3x\Big)\Big(\frac{m\omega}{\pi\hbar}\Big)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}
\end{aligned} \tag{23}$$

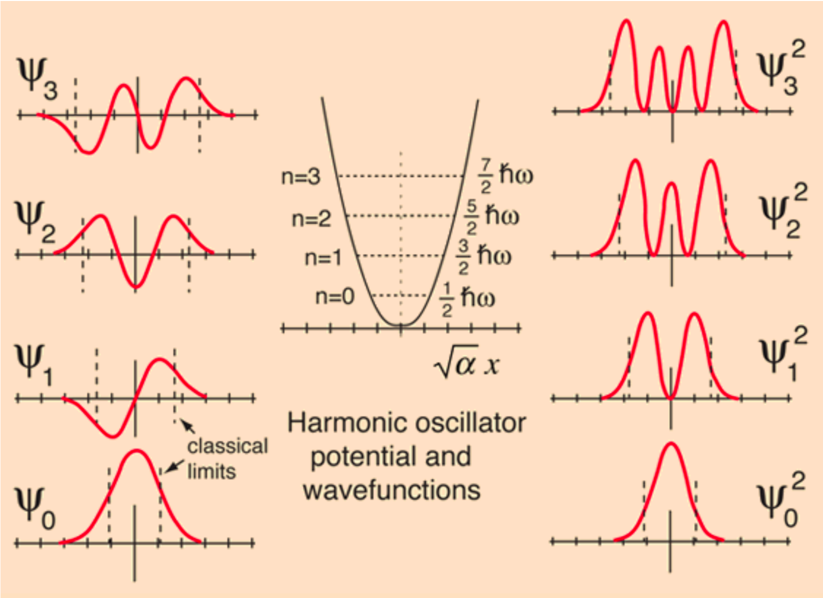
In general,

$$\psi_n(x) \;=\; \frac{1}{\sqrt{2^n n!}}\Big(\frac{m\omega}{\pi\hbar}\Big)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2} H_n(x\sqrt{\frac{m\omega}{\hbar}}) \tag{24}$$

where $H_n(y)$ is the so-called *Hermite polynomial* of order n.

The corresponding solution of time-dependent Schrödinger equation is then

$$\psi_n(x,t) \;=\; \frac{1}{\sqrt{2^n n!}}\Big(\frac{m\omega}{\pi\hbar}\Big)^{\frac{1}{4}} H_n(x\sqrt{\frac{m\omega}{\hbar}}) e^{-\frac{m\omega}{2\hbar}x^2} e^{-i\omega\left(n+\frac{1}{2}\right)t} \tag{25}$$



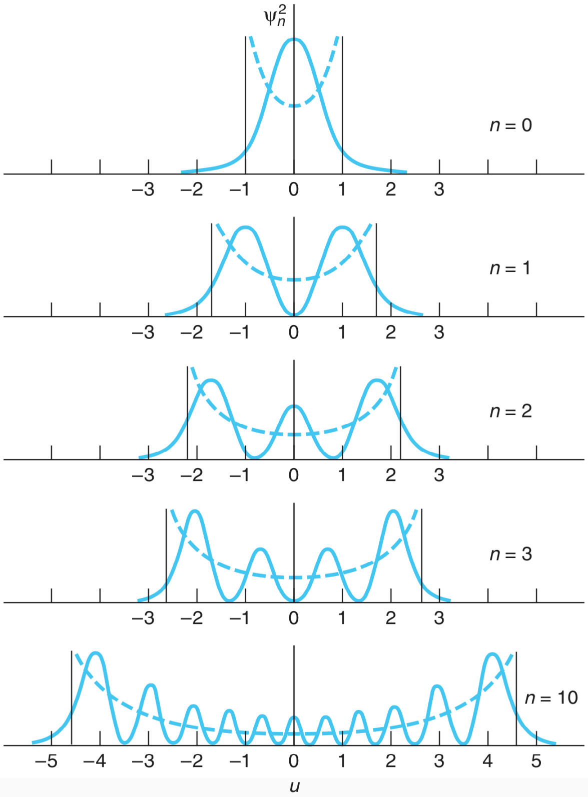


Figure 6-19 Probability density ψ_n^2 for the simple harmonic oscillator plotted against the dimensionless variable $u = (m\omega/\hbar)^{1/2}x$, for $n = 0, 1, 2, 3$, and 10. The dashed curves are the classical probability densities for the same energy, and the vertical lines indicate the classical turning points $x = \pm A$.

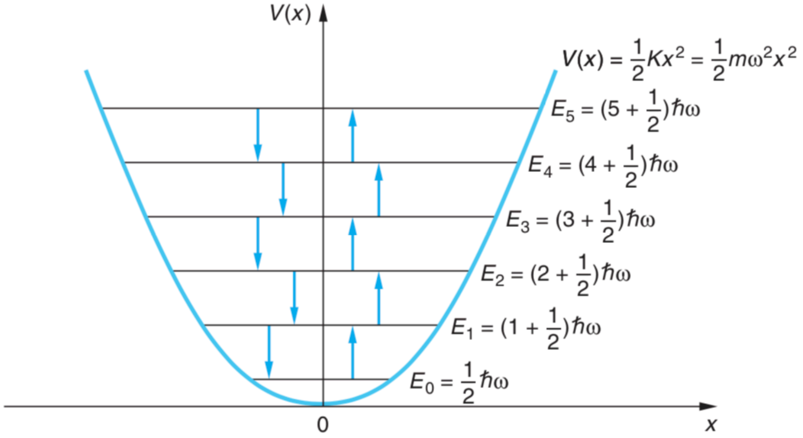


Figure 6-20 Energy levels in the simple harmonic oscillator potential. Transitions obeying the selection rule $\Delta n = \pm 1$ are indicated by the arrows (those pointing up indicate absorption). Since the levels have equal spacing, the same energy $\hbar\omega$ is emitted or absorbed in all allowed transitions. For this special potential, the frequency of the emitted or absorbed photon equals the frequency of oscillation, as predicted by classical theory.

A property of these wave functions that we will state without proof is that

$$\int_{-\infty}^{+\infty} \psi_n^* x \psi_m \, dx = 0 \quad \text{unless} \quad n = m \pm 1 \qquad \textbf{6-59}$$

This property places a condition on transitions that may occur between allowed states. This condition, called a *selection rule*, limits the amount by which n can change for (electric dipole) radiation emitted or absorbed by a simple harmonic oscillator:

> The quantum number of the final state must be 1 less than or 1 greater than that of the initial state.

This selection rule is usually written

$$\Delta n = \pm 1 \qquad \textbf{6-60}$$

Since the difference in energy between two successive states is $\hbar\omega$, this is the energy of the photon emitted or absorbed in an electric dipole transition. The frequency of the photon is therefore equal to the classical frequency of the oscillator, as was assumed by Planck in his derivation of the blackbody radiation formula. Figure 6-20 shows an energy level diagram for the simple harmonic oscillator, with the allowed energy transitions indicated by vertical arrows.