Origin of the Harmonic Oscillator Selection Rule

Figure SR-1 shows the harmonic oscillator potential and several allowed energy levels. The harmonic oscillator wave functions are

$$\psi_n(x) = C_n e^{-x^2} H_n(x) \qquad \textbf{SR-1}$$

where $x = y\sqrt{m\omega/2\hbar}$, C_n is a normalization constant, and $H_n(x)$ are the Hermite polynomials whose generating function is

$$H_n(x) = (-1)^n e^{-x^2} \frac{d^n e^{-x^2}}{dx^n} \qquad \textbf{SR-2}$$

In order to show that

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

it is first necessary to show that the $H_n(x)$ are orthogonal. We do this by considering two generating functions:

$$A(x,\alpha) = \sum_n \frac{H_n(x)}{n!}\alpha^n = e^{-x^2-(\alpha-x)^2}$$

$$B(x,\beta) = \sum_m \frac{H_m(x)}{m!}\beta^m = e^{-x^2-(\beta-x)^2} \qquad \textbf{SR-3}$$

From Equation SR-3 we can write

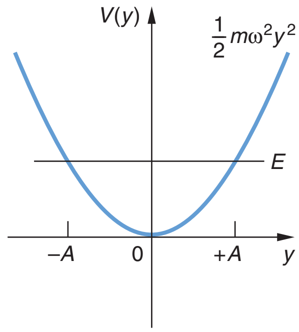
$$\int_{-\infty}^{+\infty} ABe^{-x^2}dx = \sum_n \sum_m \alpha^n \beta^m \int_{-\infty}^{+\infty} \frac{H_n(x)H_m(x)}{n!m!} e^{-x^2} dx$$

$$= \int_{-\infty}^{+\infty} e^{-\alpha^2-\beta^2+2\alpha x+2\beta x-x^2} dx = e^{2\alpha\beta} \int_{-\infty}^{+\infty} e^{-(x-\alpha-\beta)^2} d(x-\alpha-\beta)$$

$$= \sqrt{\pi}\, e^{2\alpha\beta} = \sqrt{\pi}\left(1 + \frac{2\alpha\beta}{1!} + \frac{(2\alpha\beta)^2}{2!} + \frac{(2\alpha\beta)^3}{3!} + \cdots + \frac{(2\alpha\beta)^n}{n!} + \cdots\right)$$

We can see from the coefficients of the $\alpha\beta$ terms in the expansion that $\int_{-\infty}^{+\infty} ABe^{-x^2}dx = 0$ unless $n = m$; hence

$$\int_{-\infty}^{+\infty} H_n(x)H_m(x)e^{-x^2} = 0 \qquad \text{for } n \neq m \qquad \textbf{SR-4}$$



SR-1 Potential energy function $V(y)$ for a simple harmonic oscillator such as a pendulum moving on the y axis. A possible total energy E is indicated. The points at $\pm A$ are the classical turning points, that is, the displacement positions at which a classical oscillator with energy E would reverse its direction of motion.

This result now makes it possible to evaluate integrals that involve the harmonic oscillator wave functions $\psi_n(x)$ given by Equation SR-1. For example, $P_{n\,m}$, the probability for a transition between the states n and m, is given by

$$P_{nm} = \int_{-\infty}^{+\infty} \psi_n(x)x\,\psi_m(x)\,dx$$

$$= C_nC_m\int_{-\infty}^{+\infty} H_n(x)H_m(x)e^{-x^2}x\,dx$$

Again using the generating functions A and B,

$$\int_{-\infty}^{+\infty} ABe^{-x^2}x\,dx = \sum_n\sum_m \alpha^n\beta^m\int_{-\infty}^{+\infty}\frac{H_n(x)H_m(x)}{n!m!}xe^{-x^2}dx$$

$$= e^{2\alpha\beta}\int_{-\infty}^{+\infty} e^{-(x-\alpha-\beta)^2}x\,dx$$

$$\int_{-\infty}^{+\infty} ABe^{-x^2}x\,dx = e^{2\alpha\beta}\int_{-\infty}^{+\infty} e^{-(x-\alpha-\beta)^2}(x-\alpha-\beta)\,d(x-\alpha-\beta)$$

$$+ e^{2\alpha\beta}(\alpha+\beta)\int_{-\infty}^{+\infty} e^{-(x-\alpha-\beta)^2}d(x-\alpha-\beta) \qquad \textbf{SR-5}$$

The first integral on the right side of Equation SR-5 is zero (since $e^{-(x-\alpha-\beta)^2}(x-\alpha-\beta)$ is an odd function). The second integral on the right equals $\sqrt{\pi}$, as we saw above. Expanding $e^{2\alpha\beta}$ as before, we have

$$\int_{-\infty}^{+\infty} ABe^{-x^2}x\,dx = \sqrt{\pi}\Big(\alpha + \frac{2\alpha^2\beta}{1!} + \frac{2^2\alpha^3\beta^2}{2!} + \cdots + \frac{2^n\alpha^{n+1}\beta n}{n!} + \cdots$$

$$+ \beta + \frac{2\alpha\beta^2}{1!} + \frac{2^2\alpha^2\beta^3}{2!} + \cdots + \frac{2^m\alpha^m\beta^{m+1}}{m!} + \cdots\Big) \qquad \textbf{SR-6}$$

Again, examining the coefficients of the $\alpha^n\beta^m$ terms in Equation SR-6 we see that $P_{n\,m} = 0$ except when $n = m \pm 1$. Thus, transitions between energy levels within the harmonic oscillator potential can only occur between adjacent levels, that is, for $\Delta n = \pm 1$.