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

$$\psi_n(x) = C_n e^{-\frac{x^2}{2\hbar}} H_n(x)$$

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

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

In order to show that

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

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

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

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

From Equation SR-3 we can write

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

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

$$= \sqrt{\pi} e^{2\alpha\beta} = \sqrt{\pi} \left( 1 + \frac{2\alpha\beta}{1!} + \frac{(2\alpha\beta)^2}{2!} + \frac{(2\alpha\beta)^3}{3!} + \cdots + \frac{(2\alpha\beta)^n}{n!} + \cdots \right)$$
We can see from the coefficients of the $\alpha \beta$ terms in the expansion that \[
\int_{-\infty}^{+\infty} ABe^{-x^2} \, dx = 0 \quad \text{unless } n = m; \text{ hence}
\int_{-\infty}^{+\infty} H_n(x) H_m(x) e^{-x^2} \, dx = 0 \quad \text{for } n \neq m \quad \text{SR-4}
\]

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, $P_{nm}$, the probability for a transition between the states $n$ and $m$, is given by
\[
P_{nm} = \int_{-\infty}^{+\infty} \psi_n(x) \psi_m(x) \, dx
\]
\[
= C_n C_m \int_{-\infty}^{+\infty} H_n(x) H_m(x) e^{-x^2} \, dx
\]

Again using the generating functions $A$ and $B$,
\[
\int_{-\infty}^{+\infty} ABe^{-x^2} \, dx = e^{2\alpha\beta} \int_{-\infty}^{+\infty} e^{-x^2} \, dx
\]
\[
\int_{-\infty}^{+\infty} ABe^{-x^2} \, dx = e^{2\alpha\beta} \left[ e^{-(x-\alpha-\beta)^2} (x-\alpha-\beta) \, dx \right]_{-\infty}^{+\infty}
\]
\[
\int_{-\infty}^{+\infty} ABe^{-x^2} \, dx = e^{2\alpha\beta} (\alpha + \beta) \int_{-\infty}^{+\infty} e^{-(x-\alpha-\beta)^2} \, dx
\]
\[
\int_{-\infty}^{+\infty} ABe^{-x^2} \, dx = e^{2\alpha\beta} \left[ e^{-(x-\alpha-\beta)^2} \, dx \right]_{-\infty}^{+\infty}
\]
\[
\int_{-\infty}^{+\infty} ABe^{-x^2} \, dx = e^{2\alpha\beta} (\alpha + \beta) \int_{-\infty}^{+\infty} e^{-(x-\alpha-\beta)^2} \, dx
\]
\[
\int_{-\infty}^{+\infty} ABe^{-x^2} \, dx = e^{2\alpha\beta} \left[ e^{-(x-\alpha-\beta)^2} \, dx \right]_{-\infty}^{+\infty}
\]
\[
\int_{-\infty}^{+\infty} ABe^{-x^2} \, dx = \sqrt{\pi} \left[ \alpha + \frac{2\alpha^2\beta}{1!} + \frac{2^2\alpha^3\beta^2}{2!} + \ldots + \frac{2^n\alpha^{n+1}\beta n}{n!} + \ldots \right]
\]
\[
+ \beta + \frac{2\alpha\beta^2}{1!} + \frac{2^2\alpha^2\beta^3}{2!} + \ldots + \frac{2^m\alpha^m\beta^{m+1}}{m!} + \ldots \right) \quad \text{SR-5}
\]

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
\[
\int_{-\infty}^{+\infty} ABe^{-x^2} \, dx = \sqrt{\pi} \left[ \alpha + \frac{2\alpha^2\beta}{1!} + \frac{2^2\alpha^3\beta^2}{2!} + \ldots + \frac{2^n\alpha^{n+1}\beta n}{n!} + \ldots \right]
\]
\[
+ \beta + \frac{2\alpha\beta^2}{1!} + \frac{2^2\alpha^2\beta^3}{2!} + \ldots + \frac{2^m\alpha^m\beta^{m+1}}{m!} + \ldots \right) \quad \text{SR-6}
\]

Again, examining the coefficients of the $\alpha^n\beta^m$ terms in Equation SR-6 we see that $P_{nm} = 0$ 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 $\Delta n = \pm 1$. 

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**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.