5-13. In the infrared spectrum of $^{35}$Br, there is an intense line at 2630 cm$^{-1}$. Calculate the force constant of $^{35}$Br and the period of vibration of $^{35}$Br.

\[ \nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu}} \]

\[ k = 4\pi^2 \nu^2 \mu \]

\[ k = 4\pi^2 (7.8845 \times 10^{13} \text{s}^{-1})^2 \times \frac{1.007825 \text{amu} \times 18.91259 \text{amu}}{1.007825 \text{amu} + 18.91259 \text{amu}} \times 1.660540 \times 10^{-24} \text{g/amu} \]

\[ k = 4.055 \times 10^5 \text{g/s}^2 \times 10^{-3} \frac{\text{g}}{\text{amu}} = 4.055 \times 10^5 \text{dyn cm/amu} \]

\[ k = 4.055 \times 10^5 \text{g/s}^2 \times 10^{-3} \times 9 \text{g/amu} \times \frac{9}{2630} \text{cm} \times 405.5 \text{N/m} = 3.84 \text{cm}^{-1} \]

\[ \rho = \frac{1}{\nu} = \frac{1}{7.8845 \times 10^{13} \text{s}^{-1}} = 1.268 \times 10^{-14} \text{s} \]

5-15. Verify that $\psi_1(x)$ and $\psi_2(x)$ given in Table 5.3 satisfy the Schrödinger equation for a harmonic oscillator.

\[ \psi_1(y) = \left(\frac{y^3}{\pi}\right)^{1/4} e^{-y^2/2} \]

\[ \psi_2(x) = \left(\frac{\alpha^3}{\pi}\right)^{1/4} \left(\frac{\alpha x^2 - 1}{\alpha x^2 + 1}\right)^{1/2} e^{-\alpha x^2/2} \]

\[ \frac{d^2 \psi}{dx^2} + (\beta - \alpha x^2) \psi = 0 \quad \text{where} \quad \omega = \frac{E}{m}; \quad \alpha = \frac{\hbar \omega}{\hbar}; \quad \beta = \frac{2mE}{\hbar^2} \]

\[ \frac{d\psi}{dx} = y (-y^2 e^{-y^2/2} + e^{-y^2/2}) = -y^2 e^{-y^2/2} + e^{-y^2/2} \]

\[ \frac{d^2 \psi}{dx^2} = -y^2 (-y^2 e^{-y^2/2} - 2y e^{-y^2/2} - y e^{-y^2/2}) \]

\[ \frac{d\psi}{dx} = y^3 e^{-y^2/2} - 3y e^{-y^2/2} \]

\[ \frac{d^2 \psi}{dx^2} = (y^3 e^{-y^2/2} - 3y e^{-y^2/2}) e^{-y^2/2} = 0 \]

Solution: if $\beta = 3\alpha \Rightarrow \frac{2mE}{\hbar^2} = 3\frac{m\omega}{\hbar}$ \quad \Rightarrow \quad E = \frac{3}{2}\hbar\omega \quad \checkmark
Problem 5-13  5-15, second part

\[ \psi_2 = (2 \alpha x^2 - 1) \exp[-\alpha x^2/2] \]

\[ \text{Out}(1) = e^{-x^2/2} (-1 + 2 x^2 \alpha) \]

\[ \text{In}(2) = D[\psi_2, \{x, 2\}] + (\beta - \alpha^2 x^2) \psi_2 \]

\[ \text{Out}(2) = 4 e^{-x^2/2} \alpha - 8 e^{-x^2/2} x^2 \alpha^2 + (-1 + 2 x^2 \alpha) \left( -e^{-x^2/2} \alpha + e^{-x^2/2} x^2 \alpha^2 \right) + e^{-x^2/2} (-1 + 2 x^2 \alpha) (-x^2 \alpha^2 + \beta) \]

\[ \text{In}(3) = \text{Solve}\{D[\psi_2, \{x, 2\}] + (\beta - \alpha^2 x^2) \psi_2 = 0, \beta\} \]

\[ \text{Out}(3) = \{ \{ \beta \to 5 \alpha \} \} \]
There are a number of general relations between the Hermite polynomials and their derivatives (which we will not derive). Some of these are

\[
\frac{dH_n(\xi)}{d\xi} = 2\xi H_n(\xi) - H_{n+1}(\xi)
\]

\[
H_{n+1}(\xi) - 2\xi H_n(\xi) + 2n H_{n-1}(\xi) = 0
\]

and

\[
\frac{dH_n(\xi)}{d\xi} = 2n H_{n-1}(\xi)
\]

Such connecting relations are called *recursion formulas*. Verify these formulas explicitly using the first few Hermite polynomials given in Table 5.2.

\[
H_0(\chi) = 1 \\
H_1(\chi) = 2\chi \\
H_2(\chi) = 4\chi^2 - 2 \\
H_3(\chi) = 8\chi^3 - 12\chi
\]

\[
\frac{dH_1(\chi)}{d\chi} = 2\chi H_1(\chi) - H_2(\chi) \\
2 = 2\chi(2\chi) - (4\chi^2 - 2) \\
2 = 2\chi \checkmark
\]

\[
\frac{dH_2(\chi)}{d\chi} = 2\chi H_2(\chi) - H_3(\chi) \\
8\chi = 2\chi(4\chi^2 - 2) - 8\chi^3 + 12\chi \\
8\chi = 8\chi^3 - 4\chi - 8\chi^3 + 12\chi \\
8\chi = 8\chi \checkmark
\]

\[
H_3(\chi) - 3\chi H_2(\chi) + 2\chi(H_1(\chi)) = 0 \\
8\chi^3 - 12\chi - 2\chi(4\chi^2 - 2) + 4(2\chi) \leq 0 \\
8\chi^3 - 12\chi - 8\chi^2 + 4\chi + 8\chi = 0 \checkmark
\]

\[
\frac{dH_3(\chi)}{d\chi} = 2 \times 3 H_2(\chi) \\
24\chi^2 - 12 = 6(4\chi^2 - 2) \\
24\chi^2 - 12 = 24\chi^2 - 12 \checkmark
\]
Using Mathematica (or by hand, or by any method you choose, plot psi4(x), psi5(x), |psi4(x)|^2, |psi4(x)|^2 for the harmonic oscillator. Demonstrate that psi4 and psi5 are orthogonal.

\[ \psi [\nu, x] = \left( \alpha^{(1/2)} / (\pi^{(1/2)} 2^{\nu} \nu!) \right)^{(1/2)} \text{HermiteH} [\nu, \alpha^{(1/2)} x] \exp[-\alpha x^2 / 2] \]

\[ e^{-x^2/2} \sqrt{\frac{2^{-\nu} \sqrt{\alpha}}{\nu!}} \text{HermiteH} [\nu, x \sqrt{\alpha}] \]

\[ \gamma^{1/4} \]

\[ \text{Plot}[\psi [4, x] /. \alpha \to 1, \{x, -10, 10\}] \]

\[ \text{Plot}[\psi [5, x] /. \alpha \to 1, \{x, -10, 10\}] \]
\textbf{In[7]}: \texttt{Plot[\psi[4, x]^2 / . \alpha \to 1, \{x, -10, 10\}]} \\
\textbf{Out[7]}=

\textbf{In[8]}: \texttt{Plot[\psi[5, x]^2 / . \alpha \to 1, \{x, -10, 10\}]} \\
\textbf{Out[8]}=

\textbf{In[9]}: \texttt{\int_{-\infty}^{\infty} \psi[4, x] \psi[5, x] \, dx} \\
\textbf{Out[9]}: \texttt{ConditionalExpression[0, \text{Re}[\alpha] > 0]}