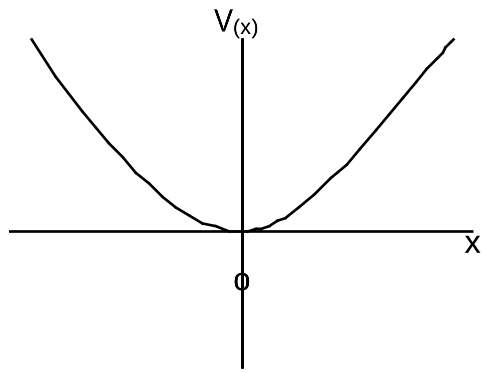
CHEM 531
LECTURE 2

<u>Harmonic Oscillator (1d)</u>

$$H = \frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2 \qquad k = m\omega^2$$

$(x = r - r_e)$



Note again $V(x) = V(-x)$. Let i_{op} be inversion operator, thus $i_{op}V(x) = V(-x)$, also $i_{op}^2 = \mathrm{I}_{op}$ (identity operator)

Note also $[i_{op}, \mathrm{H}] = 0 \quad i_{op}\mathrm{H} = \mathrm{H}_{op}$ in this case no eigs of H are eigs of i_{op}.

$$i_{op}\psi(x) = \lambda\psi(x)$$
$$i_{op^2}\psi(x) = \lambda^2\psi(x) = \psi(x) \qquad \lambda^2 = 1 \text{ so } \lambda = \pm 1$$

i.e., $\psi_g(x)$ is even, or ψ_μ is odd. Solution to H.O. are thus either even or odd wrt i_{op} .

Boundary conditions: $\psi(x) \to 0 \quad |x| \to \infty$ solutions are known.

$$\frac{d^2u}{dx^2} + \left(k^2 - \lambda^2 x^2\right)u = 0 \qquad k^2 = 2mE/\hbar^2$$
$$\lambda = m\omega/\hbar$$

Look at asymptotic form first $\lambda^2 x^2 >> k^2$

$$\left(\frac{d^2u}{dx^2} - \lambda^2 x^2\right) u_{asym} = 0$$

$$u_{asym} = e^{-\lambda x^2/2} \qquad u' = -\lambda x e^{x^2/2}$$

$$u'' = \lambda^2 x^2 e^{-\lambda x^2/2} - \lambda e^{-\lambda x^2/2} (small)$$

Try form

$$u(x) = v(x) e^{-\lambda x^2/2} \qquad v'' - 2\lambda x v' + \left(k^2 - \lambda\right) v = 0$$

Solve by series method

$$v(x) = \sum_{j=0} a_j x^j$$

$$v'' = \sum_{j=0} j(j-1) a_j x^{j-2} = a_2 + a_3 x +$$

$$v' = \sum_{j=0} j a_j x^{j-1} = a_1 + a_2 x +$$

$$\left(a_2 + a_3 x + \quad\right) - 2\lambda a_1 x - 2\lambda a_2 x^2 + \left(k^2 - \lambda\right)\left[a_0 + a_1 x + a_2 x^2 + \quad\right] \equiv 0$$

x^0 : $\qquad a_2 + \left(k^2 - \lambda\right) a_0 = 0 \qquad a_2 = \left(\lambda - k^2\right) a_0$

x^1 : $\qquad a_3 - 2\lambda a_1 + \left(k^2 - \lambda\right) a_1 = 0 \qquad a_3 = \left(3\lambda - k^2\right) a_1$

etc. in general $\qquad \boxed{a_{j+2} = \frac{\lambda(2j+1) - k^2}{(j+2)(j+1)} a_j}$

so if a_0=1 (a_1=0) get a_2, a_4 etc. – <u>even</u> solution if a_o=0

If a_0=0 and a_2=1, get a_3, a_5, etc. – <u>odd</u> solutions

This series <u>diverges</u> as $x \to \infty$ and it can be shown that it goes like $e^{\lambda x^2}$.

At some value of j (call it n) must have $\boxed{\lambda(2jn) - k^2 = 0}$ to terminate series.

Thus,

$$\frac{2mE}{\hbar^2} = \frac{m\omega}{\hbar}(2j+1) \qquad j = n$$

$$\boxed{E_n = \hbar\omega(n + 1/2)}$$ and

$$u_n(x) = \sum_{j=0}^{n} a_j x^j e^{-\lambda x^2/2}$$

and the $v_n(x)$ are Hermite polynomials.