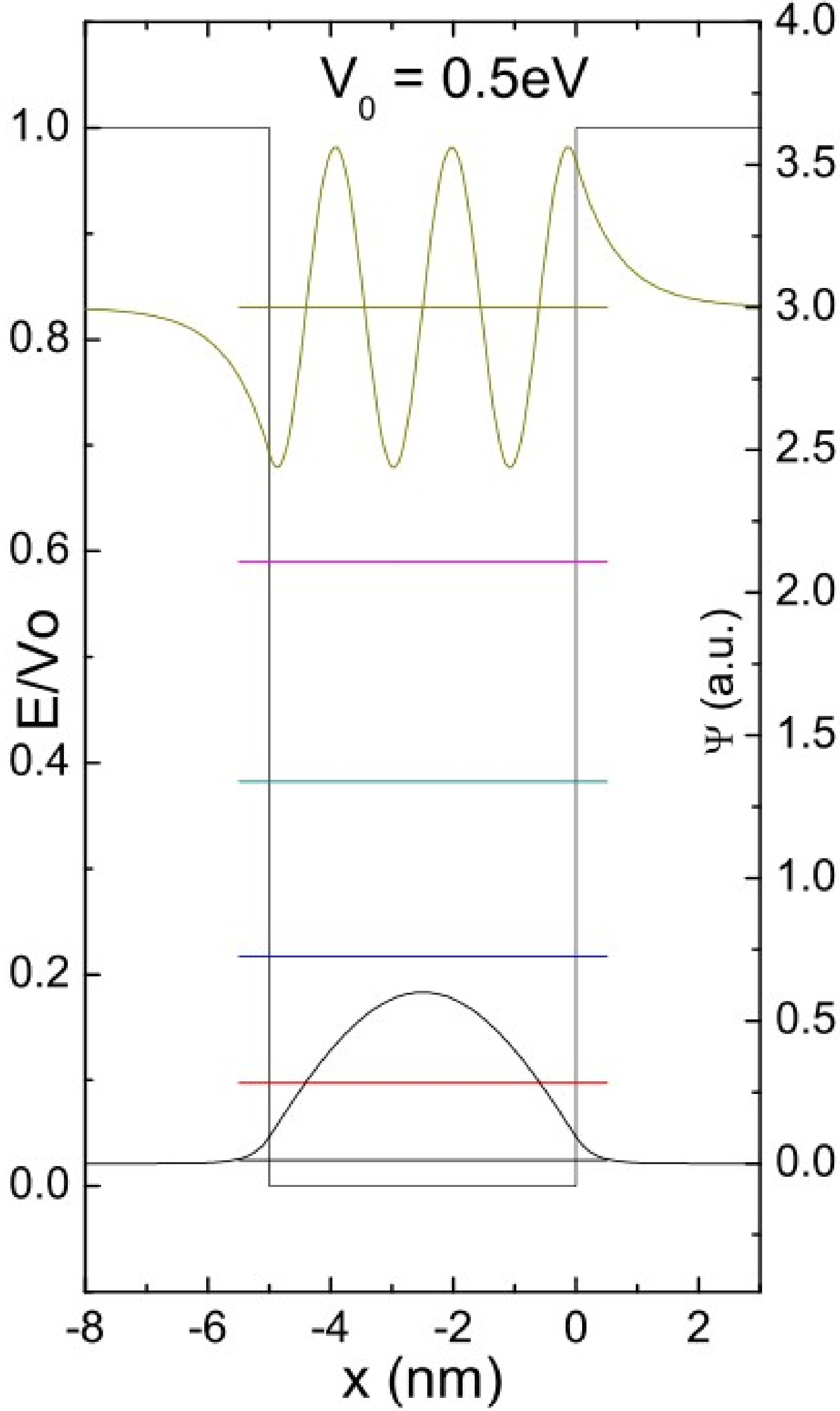
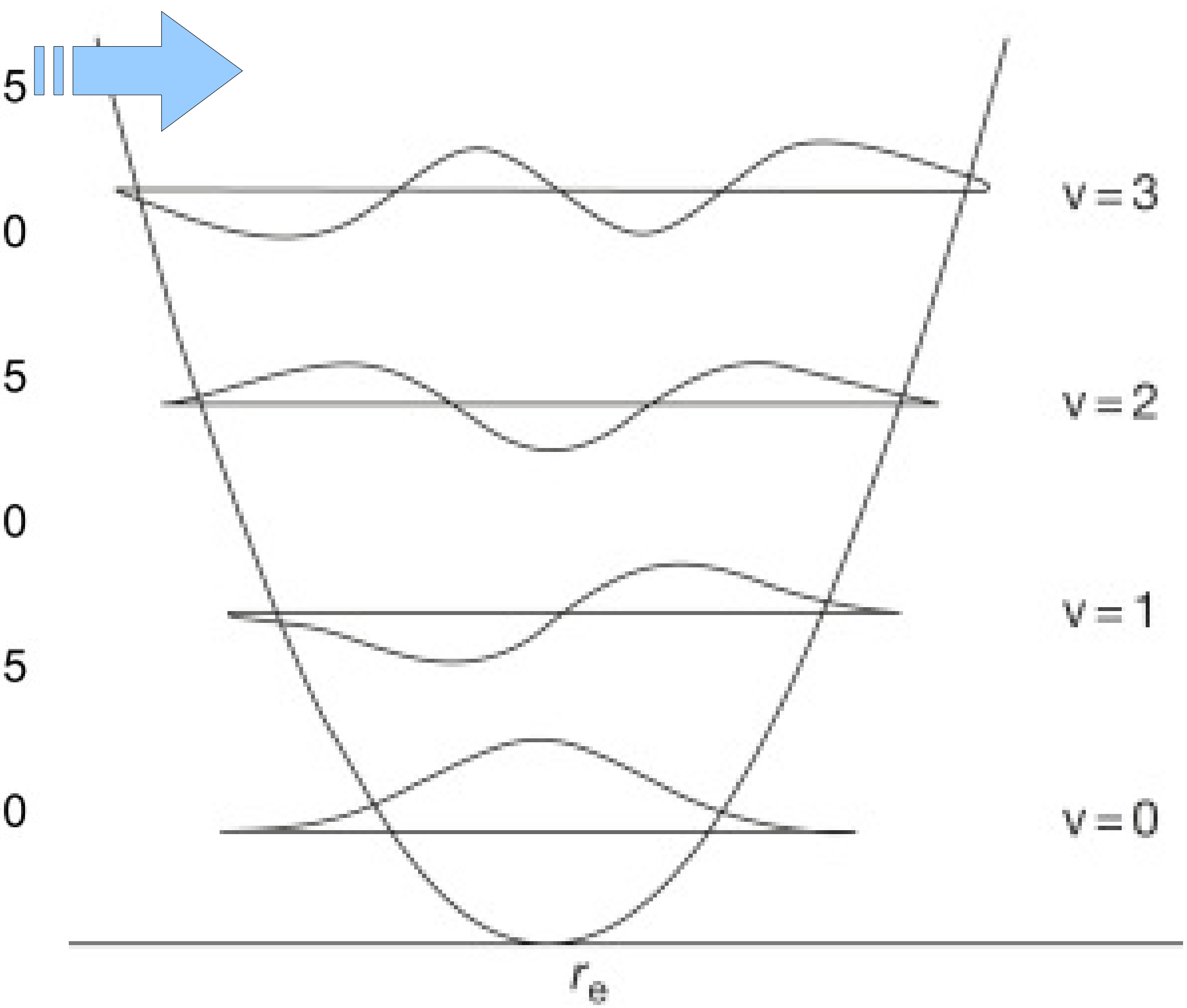
Simple Harmonic Oscillator

Extrapolating from what we know about 1D confined systems....



Reasonable expectation and educated guess about what the result might be.



Problem 8 : The Simple Harmonic Oscillator

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

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}m\omega^2 x^2\right]\psi = 0 \qquad \begin{cases} k^2 = \dfrac{2mE}{\hbar^2} \\ \alpha = \dfrac{m\omega}{\hbar} \end{cases}$$

$$\frac{d^2\psi}{dx^2} + \left[k^2 - \alpha^2 x^2\right]\psi = 0$$

Near $x \approx 0, \psi \sim \cos x$ but $\psi(x \to \infty) = ?$

We want bound states. But notice ..... $\psi \sim e^{x}$ cannot work :

$\psi \sim e^{-|x|} \to \psi'(0+) \neq \psi'(0-)$ How about $\psi \sim e^{-x^2}$?

Problem 8 : 1D-SHO : Verify if $\psi \sim e^{-\beta x^2}$ works ?

$$\psi = e^{-\beta x^2} \Rightarrow \psi' = -2\beta x e^{-\beta x^2} \Rightarrow \psi'' = \left(4\beta^2 x^2 - 2\beta\right) e^{-\beta x^2}$$

$$\psi'' + \left(k^2 - \alpha^2 x^2\right)\psi = \left(4\beta^2 x^2 - 2\beta\right) e^{-\beta x^2} + \left(k^2 - \alpha^2 x^2\right) e^{-\beta x^2}$$

Can this be zero for all values of x ?

Only if $\alpha^2 = 4\beta^2$ & $k^2 = 2\beta$ $\Rightarrow \beta = \frac{\alpha}{2}$ $K^2 = 2\beta = \alpha$

and

So we get ONE solution ! : $\boxed{E = \frac{\hbar\omega}{2} \quad : \quad \psi = A e^{-\frac{\alpha x^2}{2}}}$

This is NOT the only solution. But the behaviour for large x will look very similar to this. So we try to factor out this part.

Solving a differential equation is often done this way. You figure out one part of the behaviour and try to simplify the whole equation by taking away the "known" part.

Problem 8 : 1D-SHO : Eliminate one more constant using $u^2 = \alpha x^2$

$$u = \sqrt{\alpha}\, x \quad \Rightarrow \quad \frac{d\psi}{dx} = \sqrt{\alpha}\frac{d\psi}{du} \quad \rightarrow \quad \frac{d^2\psi}{dx^2} = \alpha \frac{d^2\psi}{du^2}$$

$$\frac{d^2\psi}{dx^2} + \left[k^2 - \alpha^2 x^2\right]\psi = 0 \quad \rightarrow \quad \boxed{\frac{d^2\psi}{du^2} + \left[\lambda - u^2\right]\psi = 0}$$

$$\lambda \equiv \frac{k^2}{\alpha} \equiv \frac{2E}{\hbar\omega}$$

We already know one solution....

Factor out the asymptotic part. $\psi(u) = f(u)\, e^{-\frac{u^2}{2}}$

We expect $f(u)$ will satisfy a simpler equation from which we will be able to get all the others....

Problem 8 : 1D-SHO : factoring out the asymptotic part

$$\psi(u) = f(u)e^{-u^2/2}$$

$$\psi' = f'e^{-u^2/2} - f\,u\,e^{-u^2/2}$$

$$\psi'' = f''e^{-u^2/2} - 2f'u\,e^{-u^2/2} + f(u^2-1)e^{-u^2/2}$$

$$\Rightarrow \left[f'' - 2uf' + (u^2-1)f\right]e^{-u^2/2} + (\lambda - u^2)f\,e^{-u^2/2} = 0$$

$$= \boxed{f'' - 2uf' + (\lambda-1)f = 0}$$

We already know one trivial solution of the equation from what we have done before. Which is f = const, which requires $\lambda = 1$

Let's try some guesses ! Can $f(u) = u$ work as a solution ?
Obviously a dfferent value of λ will be needed .

Problem 8 : 1D-SHO : Solving the remaining part

$$f'' - 2u f' + (\lambda - 1) f = 0 \qquad \text{Q: does } f(u) = u \text{ work ?}$$

$$0 - 2u + (\lambda - 1) u = 0 \quad \Rightarrow \quad \lambda = 3 \quad \Rightarrow \quad E = \frac{3}{2}\hbar\omega$$

So we now have two solutions. Expectedly the lower solution was even the higher one odd.

To get all the solutions we need to work out the method of "Series solutions" . But let us try another one before that.....

$$f'' - 2u f' + (\lambda - 1) f = 0 \qquad \text{Q: does } f(u) = u^2 \text{ work ?}$$

$$2 - 4u^2 + (\lambda - 1) u^2 \neq 0 \quad \Rightarrow \text{try } f = u^2 + c_0$$

$$2 + (\lambda - 1) c_0 + \underbrace{(\lambda - 5)}_{=0} u^2 = 0 \quad \Rightarrow E = \frac{5}{2}\hbar\omega \quad \& \quad f = u^2 - \frac{1}{2}$$

Problem 8 : 1D-SHO : Series solution of $f''-2u\,f'+(\lambda-1)\,f=0$

Assume a general polynomial series (could be infinite)

$$f(u)=\sum_0^\infty c_n u^n \;\Rightarrow\; \begin{cases} f' = \sum_1^\infty c_n n\,u^{n-1} \\ f'' = \sum_2^\infty c_n n(n-1)\,u^{n-2} \end{cases}$$

also has constant terms

Notice that the lower limit of the sum changes !

$$f''-2u\,f'+(\lambda-1)\,f=0$$

$$\sum_2^\infty c_n n(n-1)u^{n-2}-2\sum_1^\infty c_n n\,u^n+(\lambda-1)\sum_0^\infty c_n u^n=0$$

This is a polynomial that is needs to be zero for all values of the variable u $\rightarrow$ the coefficients of every power must individually vanish. The series may have finite or infinite number of terms.

Problem 8 : 1D-SHO : Series solution of $f''-2u\,f'+(\lambda-1)f=0$

$$f''-2u\,f'+(\lambda-1)f=0$$

$$\sum_{2}^{\infty} c_n n(n-1)u^{n-2} \;-\; 2\sum_{1}^{\infty} c_n n\,u^n \;+\; (\lambda-1)\sum_{0}^{\infty} c_n u^n=0$$

Equating the coefficients of each power to zero

$$\begin{array}{lcllllll}
u^0 & : & 2.1.c_2 & + & 0 & + & (\lambda-1)c_0=0 \\
u^1 & : & 3.2.c_3 & - & 2c_1 & + & (\lambda-1)c_1=0 \\
u^2 & : & 4.3.c_4 & - & 2.2.c_2 & + & (\lambda-1)c_2=0 \\
u^3 & : & 5.4.c_5 & - & 2.3.c_3 & + & (\lambda-1)c_3=0 \\
u^4 & : & 6.5.c_6 & - & 2.4.c_4 & + & (\lambda-1)c_4=0 \\
 & & & & \vdots & &
\end{array}$$

2^{nd} order diff eqn $\Rightarrow$ TWO arbitrary coefficients

Choose c_0 & c_1 to be those two

Problem 8 : 1D-SHO : Series solution of $f'' - 2u f' + (\lambda - 1) f = 0$

$$f'' - 2u f + (\lambda - 1) f = 0$$

$$\sum_{2}^{\infty} c_n n(n-1) u^{n-2} \; - \; 2\sum_{1}^{\infty} c_n n u^n \; + \; (\lambda - 1)\sum_{0}^{\infty} c_n u^n = 0$$

$$u^0 \;:\; 2.1.c_2 \; + \; (\lambda-1)c_0 = 0$$

$$u^1 \;:\; 3.2.c_3 \; + \; (\lambda-3)c_1 = 0$$

$$u^2 \;:\; 4.3.c_4 \; + \; (\lambda-5)c_2 = 0$$

$$u^3 \;:\; 5.4.c_5 \; + \; (\lambda-7)c_3 = 0$$

$$u^4 \;:\; 6.5.c_6 \; + \; (\lambda-9)c_4 = 0$$

$$\boxed{\lambda = \frac{2E}{\hbar\omega}}$$

already a sol$^{n.}$

$$\boxed{\lambda = 1 \quad c_0 \neq 0} \;\Rightarrow\; c_2 = 0 \;\Rightarrow\; c_4 = 0 \;\Rightarrow\; c_6 = 0 \ldots.$$

But what about $c_1, c_3, c_5 \ldots..?$ Assume $c_1 \neq 0$

Problem 8 : 1D-SHO : $f''-2uf'+(\lambda-1)f=0$: possible choice of λ, c_0, c

$$\left.\begin{aligned} c_1 &= 1 \\ c_3 &= \frac{c_1}{3}=\frac{1}{3} \\ c_5 &= \frac{c_3}{5}=\frac{1}{5}\frac{1}{3} \\ c_7 &= \frac{c_5}{7}=\frac{1}{7}\frac{1}{5}\frac{1}{3} \\ .... &= .... \end{aligned}\right\} \Rightarrow \psi=\left[c_0+c_1\boxed{\left(u+\frac{u^3}{3}+\frac{u^5}{5.3}+\frac{u^7}{7.5.3}+....\right)}\right]e^{-u^2/2}$$

If $\lambda=1$ & $c_1\neq 0$ (say $c_1=1$)

$\lambda = 1 \quad 3 \quad 5 \quad 7 \quad 9 \quad 11$

$c_n = 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5$

The part in the (.........) diverges too fast.

...faster than $e^{-u^2/2}$ can force convergence

$\rightarrow$ We cannot have this part in a normalizable bound state

$\rightarrow \lambda=1,3,5,7......$ are allowed because the series will terminate

$\rightarrow$ If $\lambda\neq 1,3,5,7$ same problem with convergence will appear

Problem 8 : 1D-SHO : $f'' - 2u f' + (\lambda - 1) f = 0$: possible choice of λ , c_0, c

To get a convergent series we need

$$\lambda = 1,3,5,7,9 \Rightarrow E = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$\left.\begin{array}{l} c_0 \neq 0 \\ c_1 = 0 \end{array}\right\} \Rightarrow f(u) = c_0 + c_2 u^2 + c_4 u^4 + \ldots$$

OR

$$\left.\begin{array}{l} c_1 \neq 0 \\ c_0 = 0 \end{array}\right\} \Rightarrow f(u) = c_1 u + c_3 u^3 + c_5 u^5 + \ldots$$

Notice that the alternation of odd-even wavefunctions.

It is not an assumption. It appears naturally

We can now generate the solutions one by one

Problem 8 : 1D-SHO : $f'' - 2u f + (\lambda - 1) f = 0$: Hermite polynomials

$$\lambda = 1 \quad : \quad c_0 = 1 \quad \rightarrow \quad c_{2,} c_{4,} c_{6.} ..0$$

$$\lambda = 3 \quad : \quad c_1 = 1 \quad \rightarrow \quad c_{3,} c_{5,} c_{7.} ..0$$

$$\lambda = 5 \quad : \quad c_0 = 1 \quad \rightarrow \quad c_2 = -2 \quad \rightarrow c_{4,} c_{6.} ...0$$

$$\lambda = 7 \quad : \quad c_1 = 1 \quad \rightarrow \quad c_3 = -\frac{2}{3} \quad \rightarrow c_{5,} c_{7.} ...0$$

$$\lambda = 9 \quad : \quad c_0 = 1 \quad \rightarrow \quad c_2 = -4 \rightarrow c_4 = \frac{4}{3} \quad \rightarrow c_{6,} c_{8.} ...0$$

$$\boxed{\Rightarrow H_4(x) = \frac{4}{3} x^4 - 4x^2 + 1 \quad \rightarrow \quad 16x^4 - 48x^2 + 12 \\ \text{Normalisation for } H_n \text{ : Leading power} = 2^n = 4}$$

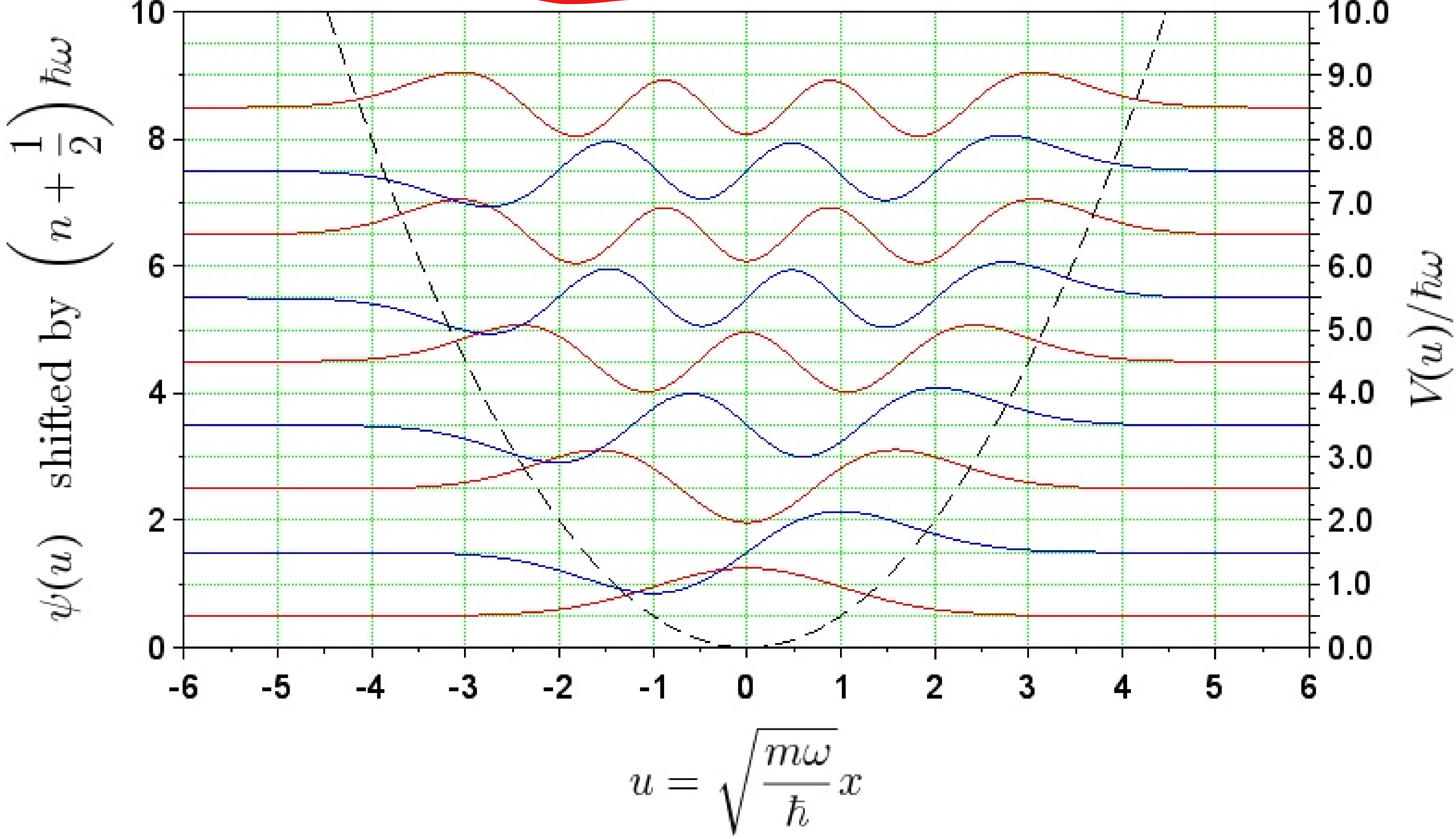
Problem 8 : 1D-SHO : First few Hermite Polynomials

$$
\begin{aligned}
H_0(x) &= 1 \\
H_1(x) &= 2x \\
H_2(x) &= 4x^2 - 2 \\
H_3(x) &= 8x^3 - 12x \\
H_4(x) &= 16x^4 - 48x^2 + 12 \\
H_5(x) &= 32x^5 - 160x^3 + 120x \\
H_6(x) &= 64x^6 - 480x^4 + 720x^2 - 120 \\
H_7(x) &= 128x^7 - 1344x^5 + 3360x^3 - 1680x \\
H_8(x) &= 256x^8 - 3584x^6 + 13440x^4 - 13440x^2 + 1680
\end{aligned}
$$

$$\boxed{e^{2xt - t^2} = \sum_{0}^{\infty} H_n(x) \frac{t^n}{n!}}$$

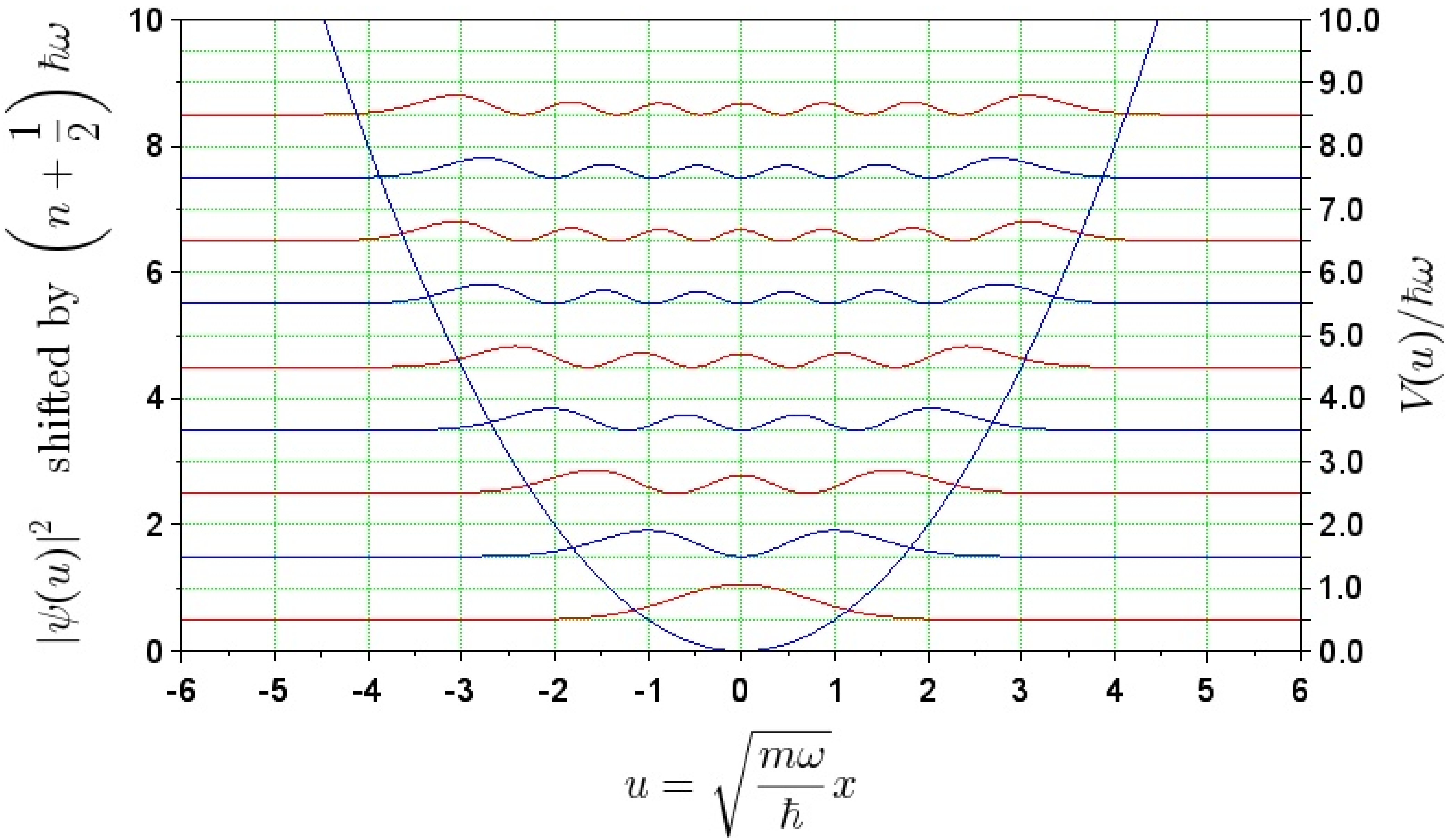
Problem 8 : 1D-SHO : complete wavefunctions and normalization

$$\psi(u,t) = \frac{1}{\sqrt{2^n n!}} \pi^{-1/4} e^{-u^2/2} H_n(u) e^{-i E_n t/\hbar} \qquad \text{where} \quad u = \sqrt{\frac{m\omega}{\hbar}}$$



Problem 8 : 1D-SHO : complete wavefunctions and normalization

$$|\psi(u,t)|^2 = \frac{1}{2^n n!}\pi^{-1/2} e^{-u^2} |H_n(u)|^2 \qquad \text{where} \quad u = \sqrt{\frac{m\omega}{\hbar}}$$



Problem 8 : 1D-SHO : Orthognality and completeness

ORTHOGONALITY of eigenstates $\Rightarrow \int_{-\infty}^{\infty} \psi_n^* \psi_m \, dx = \delta_{mn}$

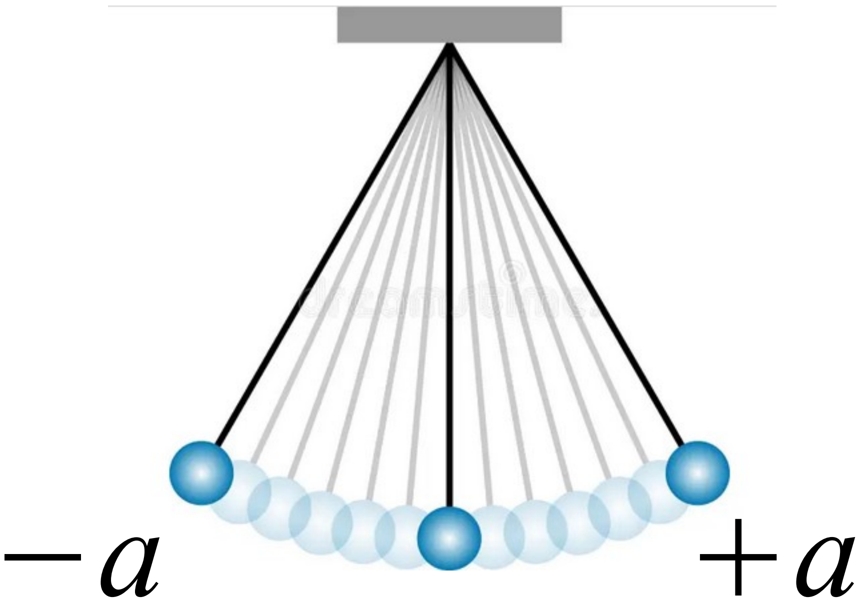
COMPLETENESS means that any function $f(x)$

can be expanded as $f(x) = \sum_{n=0}^{\infty} c_n H_n e^{-x^2/2}$

where c_n are constant co-efficients depending on $f(x)$

This is just like Fourier expansion using a different basis.
Can you figure out how to calculate each c_n ?

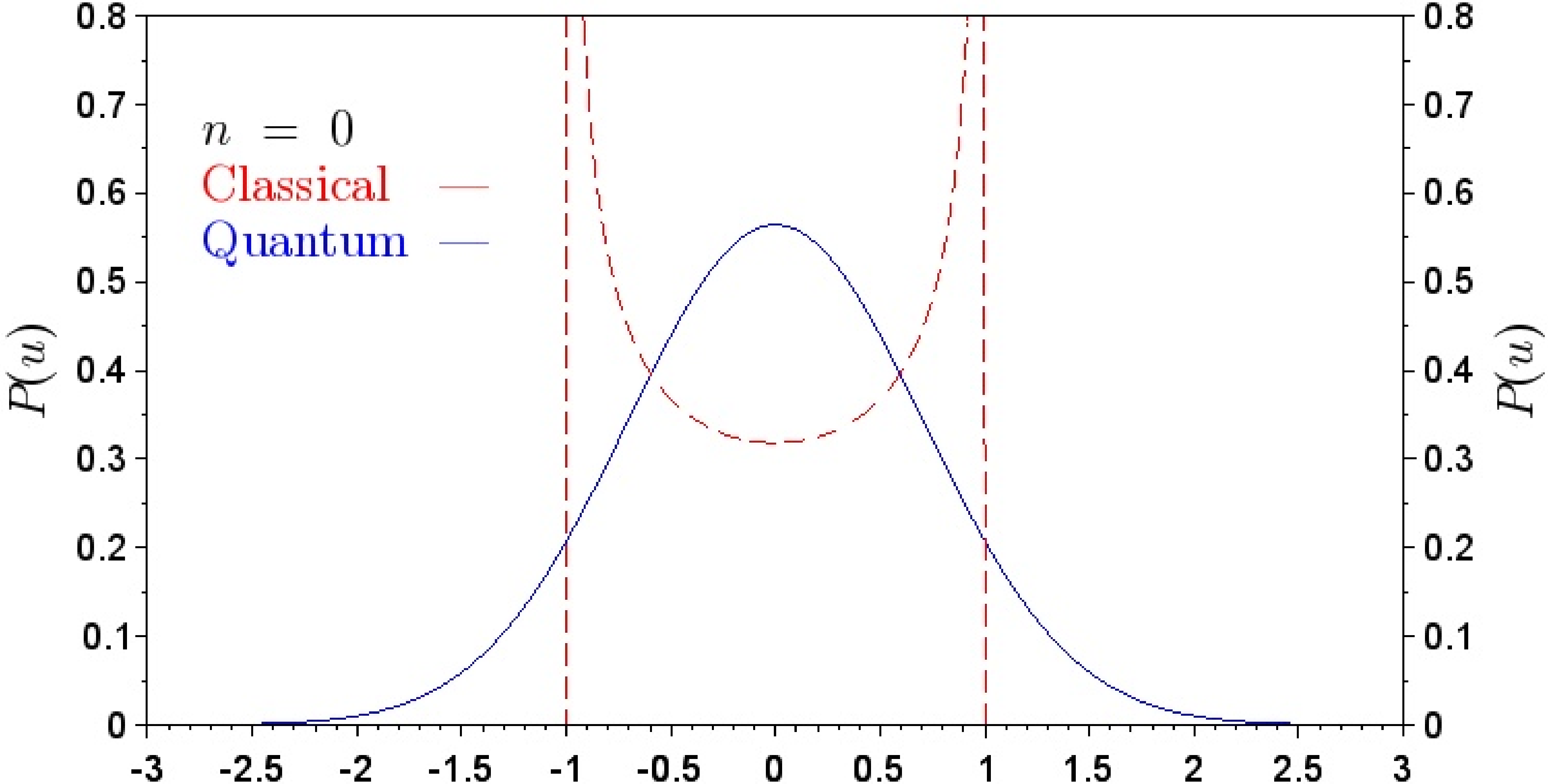
A Classical probability problem



A pendulum keeps oscillating between $-a < x < a$. A camera snaps a picture. What is the probability in the snapshot the bob will be between x to $x+dx$?

$$P(x)\,dx = \frac{2}{T}\frac{dx}{v} = \frac{1}{\pi}\frac{dx}{\sqrt{a^2 - x^2}} \qquad \text{.... why ?}$$

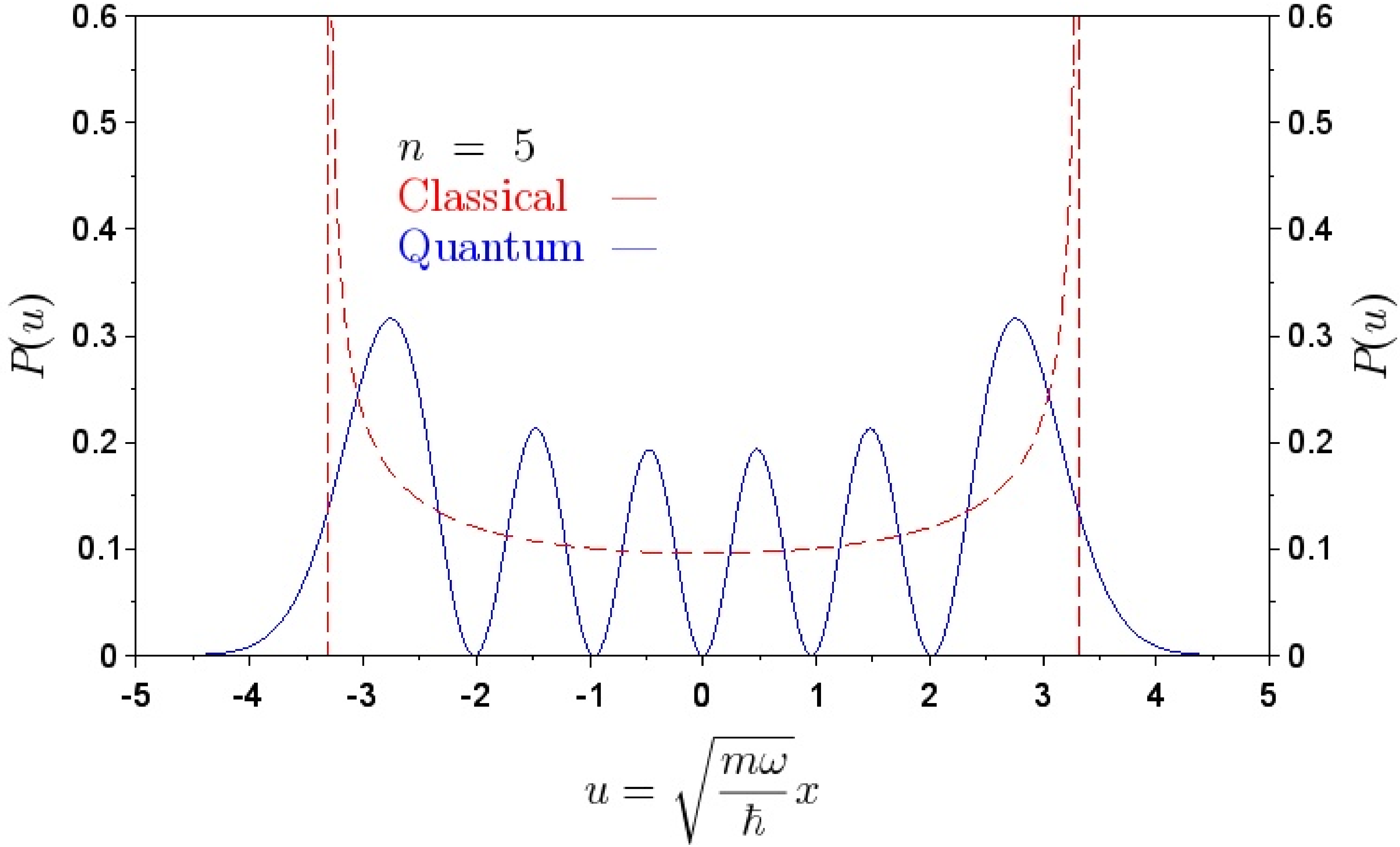
Problem 8 : 1D-SHO : Classical and Quantum location probabilities



$$u = \sqrt{\frac{m\omega}{\hbar}}x$$

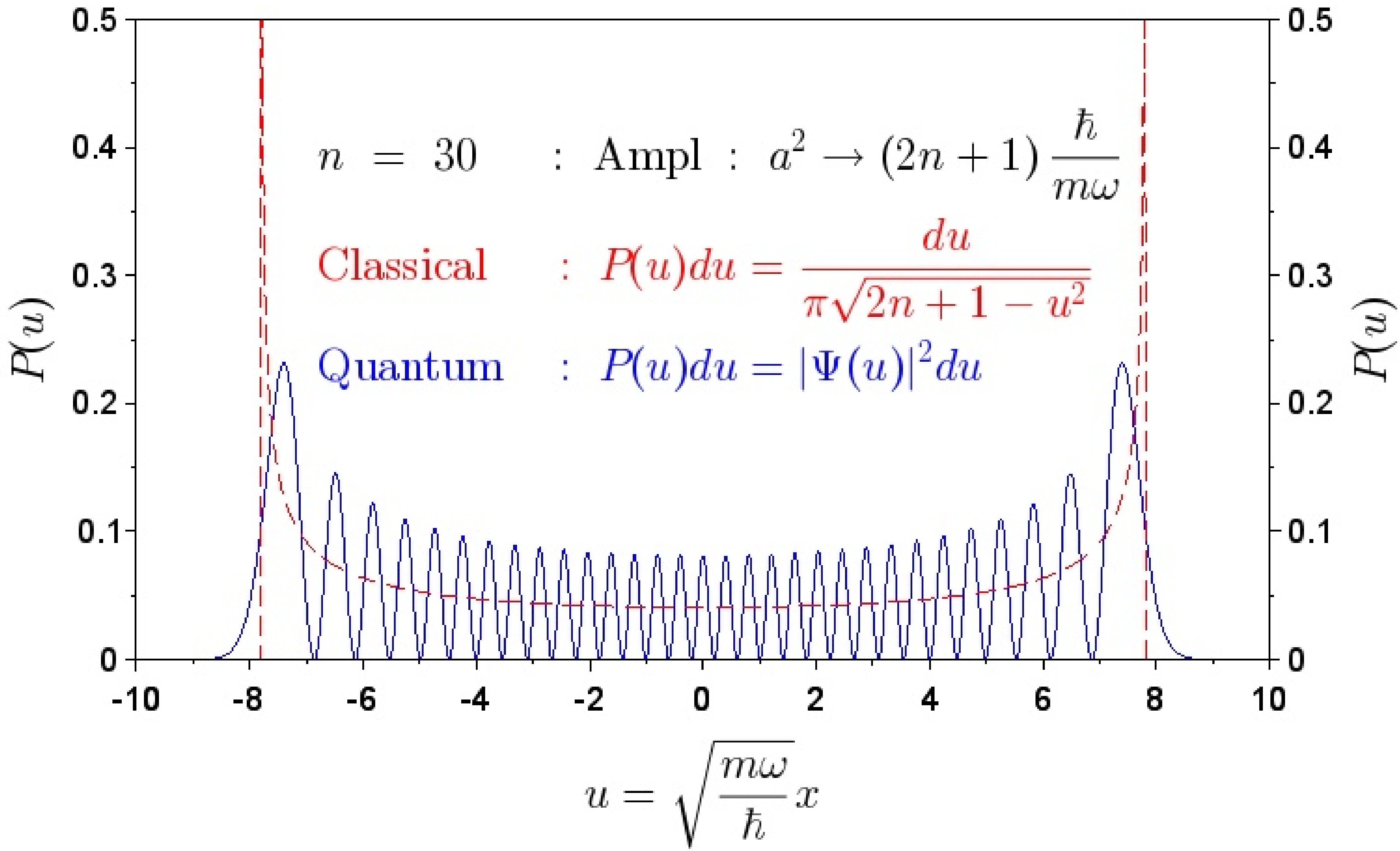
Small quantum number → classical and quantum nature are very different

Problem 8 : 1D-SHO : Classical and Quantum location probabilities



intermediate quantum number → classical and quantum nature are different

Problem 8 : 1D-SHO : Classical and Quantum location probabilities



Large quantum number → classical and quantum nature have similarities.
This is a generic fact, usually true for all quantum systems

1D-SHO : Making use of this model for diatomic molecules

What holds diatomic molecules like H_2, O_2, N_2, CO, NO, HCl etc. together? Such a potential *must* be attractive at large distances and repulsive at very small distances (*why* ?). A very commonly used model is called the Lennard Jones potential.

$$V(r)=4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right]$$

First calculate the equilibrium separation and approximate *V(r)* by a parabola at that potential minima. Here *r* is the relative co-ordinate.

→ We can now "quantise" the problem by first calculating the frequency of small oscillations about the minima.

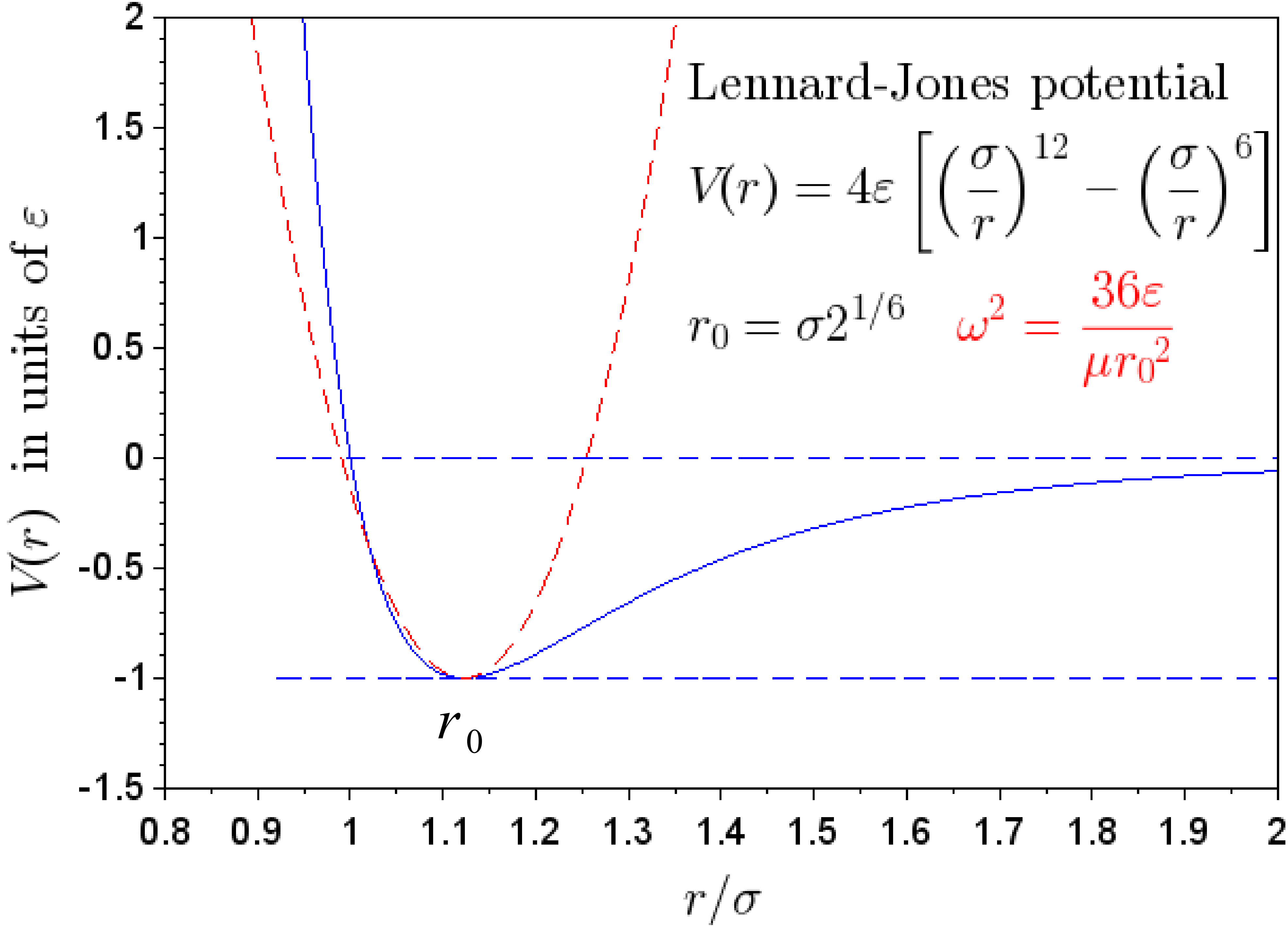
→ Once the natural frequency is known......we can calculate the internal parameters. How ?

Molecular spectroscopy !

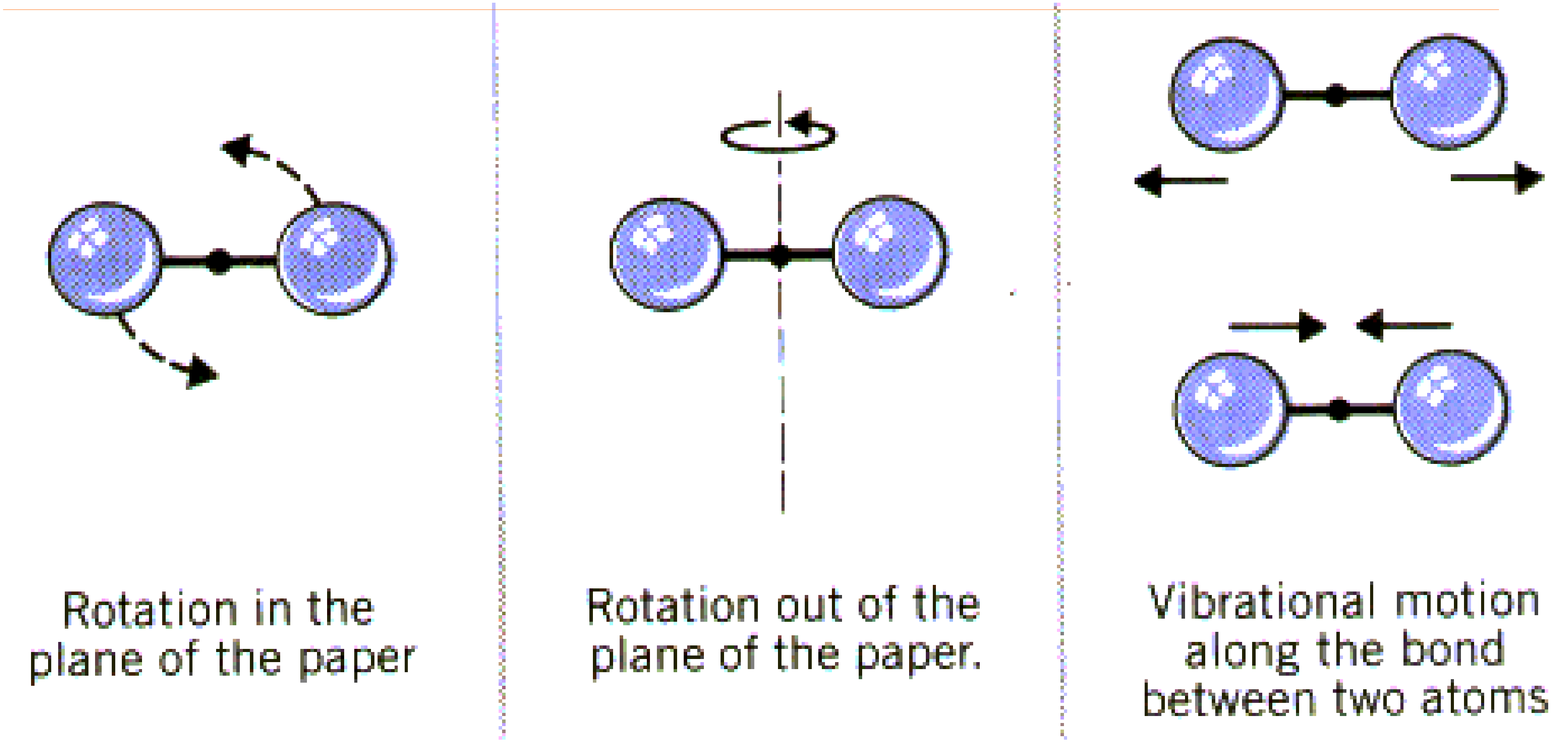
Vibrational spectra → transitions between SHO states (~infra-red)

Rotational spectra → transitions between rotational states (~microwave)

1D-SHO : Making use of this model for diatomic molecules



The molecule will rotate and vibrate.....

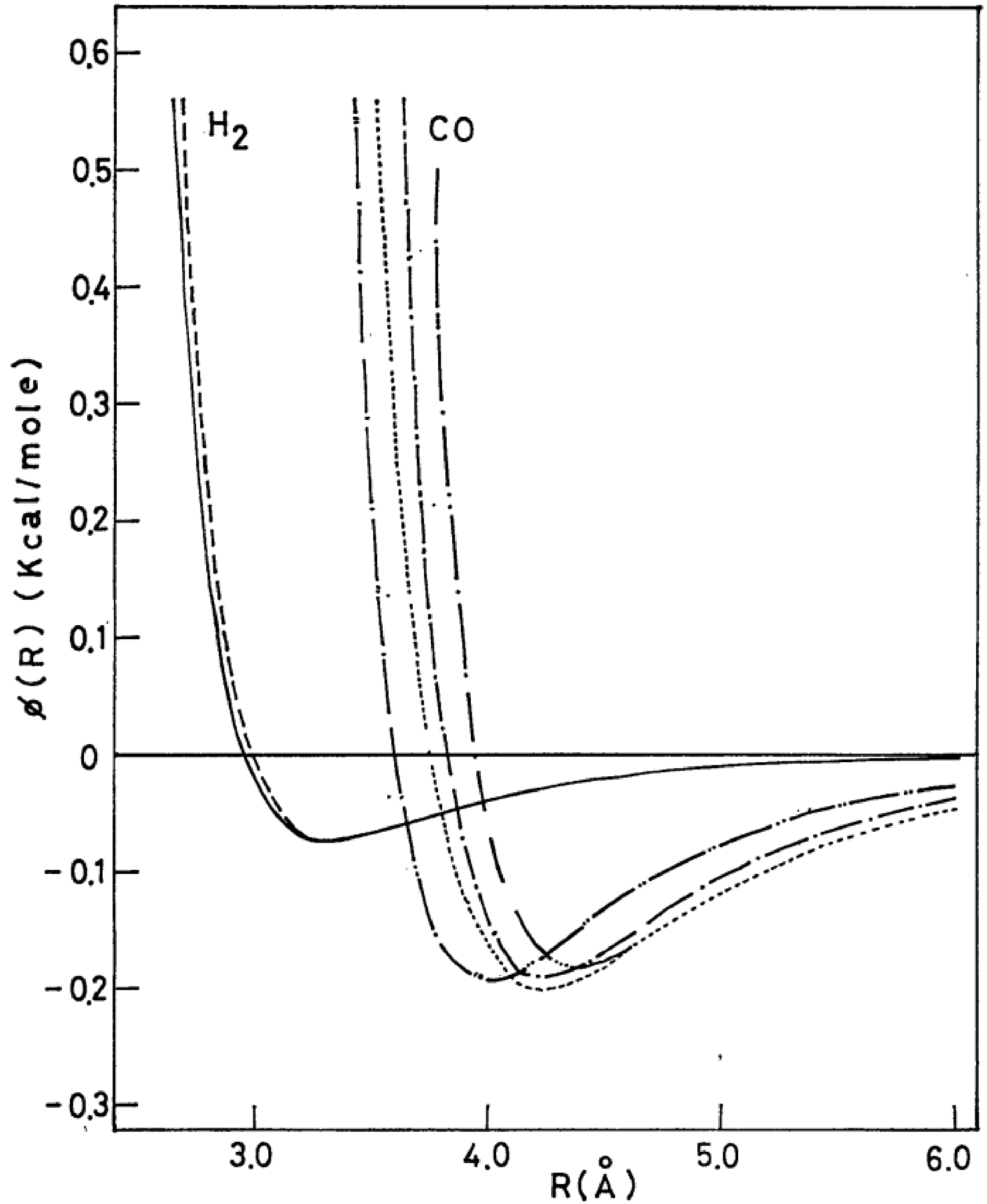


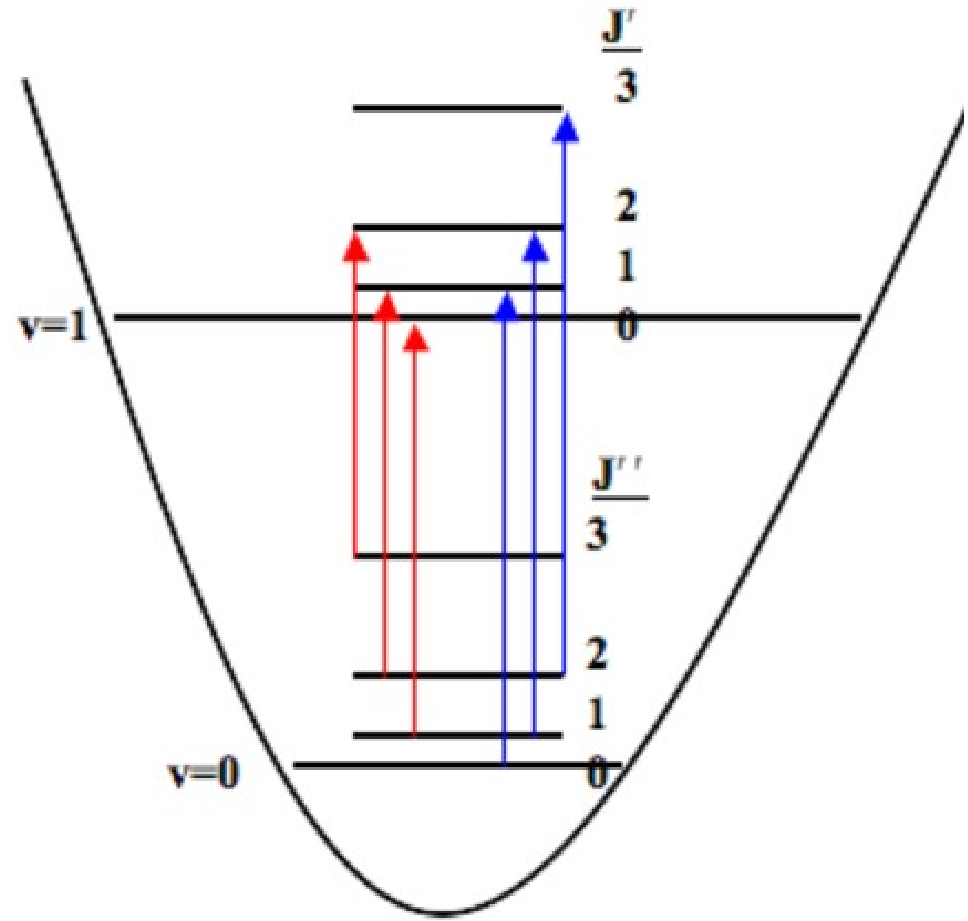
Rotational levels → small spacing (usually microwave frequencies). It is a measure of the rotational inertia & the bond length of the molecule.

Vibrational levels → larger spacing. Measure of the spring constant. Usually in infra-red frequencies

Together they give a good picture of the interaction between the two atoms of the molecule

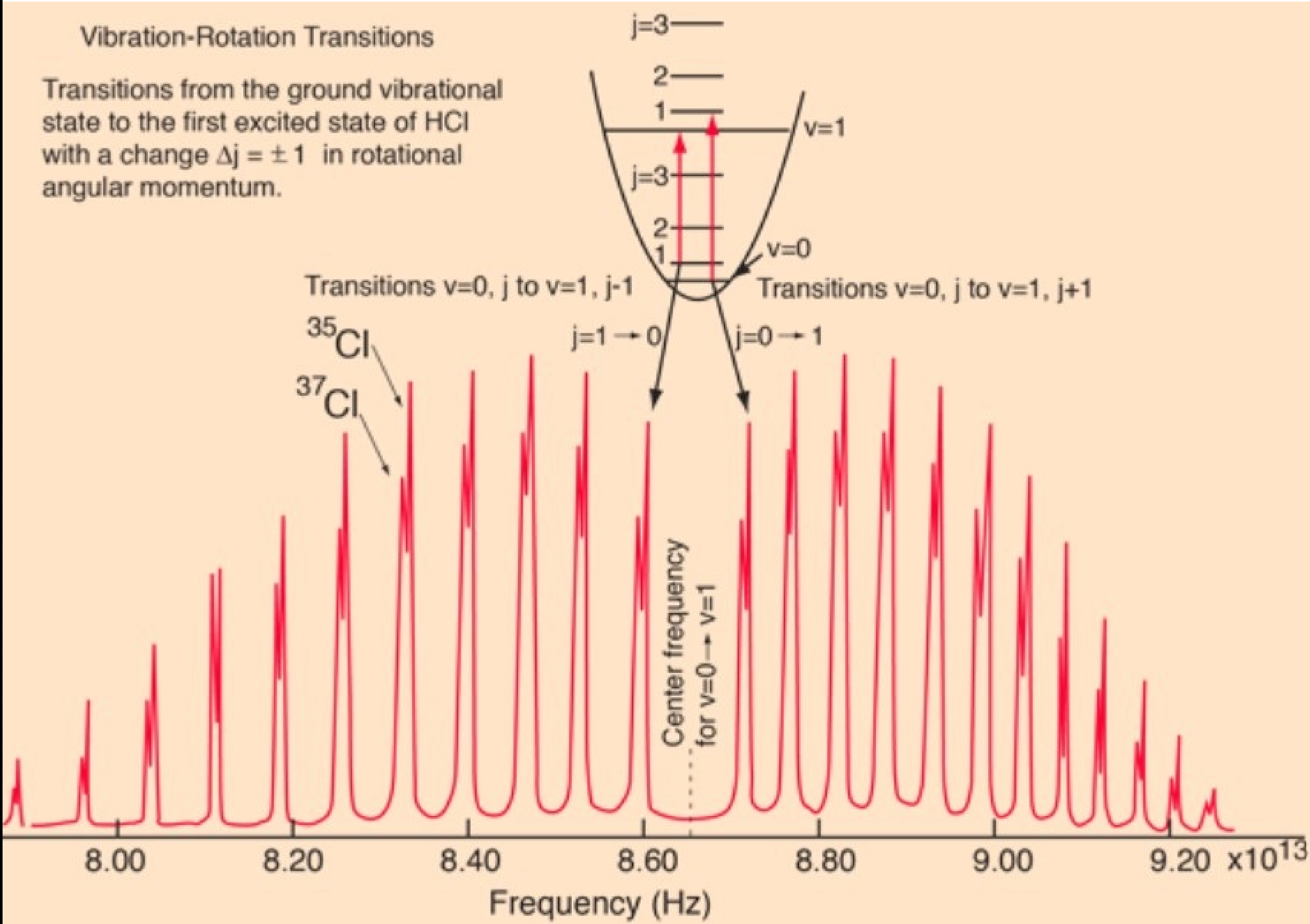
1D-SHO : Making use of this model for diatomic molecules





What would one see in the spectrum ?

What does Energy conservation tell us for e^--Xray scattering?



http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/vibrot2.html#c1

Formulating problems in 2D and 3D

Extending to 2D and 3D

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right)+\frac{1}{2}m\omega^2\left(x^2+y^2\right)\psi = E\psi$$

Separate the variables $\psi(x,y) = f(x)g(y)$

Then

$$\left[-\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2}+\frac{1}{2}m\omega^2x^2f\right]g + \left[-\frac{\hbar^2}{2m}\frac{d^2 g}{dy^2}+\frac{1}{2}m\omega^2y^2g\right]f = Efg$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2}+\frac{1}{2}m\omega^2x^2f\right]\frac{1}{f} + \left[-\frac{\hbar^2}{2m}\frac{d^2 g}{dy^2}+\frac{1}{2}m\omega^2y^2g\right]\frac{1}{g} = E_1+E_2$$

Then

$$\left[-\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2}+\frac{1}{2}m\omega^2x^2f\right]\frac{1}{f}-E_1 = -\left[\left[-\frac{\hbar^2}{2m}\frac{d^2 g}{dy^2}+\frac{1}{2}m\omega^2y^2g\right]\frac{1}{g}-E_2\right]$$

LHS is function of x only : *RHS* is function of y...

Extending to 2D and 3D : General strategy

A function of x ONLY = A function of y ONLY for all values of (x,y)

This is only possible if BOTH the functions are equal to some constant.

This is the key to "separation of variables"

Starting from a **partial differential equation**, we derive two (for 2D) or three (for 3D) **ordinary differential equations**.

There is no guarantee that this will be possible. But for many practical situations it TURNS OUT to be POSSIBLE.

Continue with the Harmonic oscillator....

Extending to 2D and 3D : General strategy

$$\left[-\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2}+\frac{1}{2}m\omega^2 x^2 f\right]\frac{1}{f}-E_1 \quad = \quad 0$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2 g}{dy^2}+\frac{1}{2}m\omega^2 y^2 g\right]\frac{1}{g}-E_2 \quad = \quad 0$$

$$\Rightarrow \quad E=\hbar\cancel{\omega}\left[\omega_1\left(n_x+\frac{1}{2}\right)+\omega_2\left(n_y+\frac{1}{2}\right)\right]$$

The extension to 3D should be obvious.....

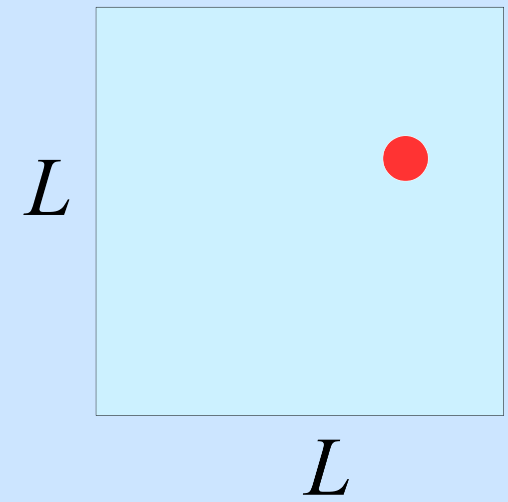
Same E can arise from different (n_x, n_y) combinations

This is called DEGENERACY

The particle in the box : in 2D and 3D

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}\right) = E\psi$$

$$\text{Try } \psi(x,y) = f(x)g(y)$$



$$\left[-\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2}\right]g + \left[-\frac{\hbar^2}{2m}\frac{d^2 g}{dy^2}\right]f = Efg$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2 f}{dx^2}\right]\frac{1}{f} + \left[-\frac{\hbar^2}{2m}\frac{d^2 g}{dy^2}\right]\frac{1}{g} = E$$

$$\Rightarrow \begin{cases} \psi(x,y) = \left(\sqrt{\frac{2}{L}}\right)^2 \sin\left(\frac{n_x \pi x}{L}\right)\sin\left(\frac{n_y \pi y}{L}\right) \\ E = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^{\,2}+n_y^{\,2}\right) \qquad n_x, n_y = 1,2,3\ldots\ldots \end{cases}$$

The particle in the box : in 2D/3D....how many states between E to $E + dE$?

n_x	n_y	$n_x^2 + n_y^2$
1	1	2
2	1	5
1	2	5
2	2	8
3	1	10
1	3	10
3	2	13
2	3	13
4	1	17
1	4	17
3	3	18
4	2	20
2	4	20

The smaller values can be tabulated by counting the numbers one by one.

${}^{n+r-1}C_{r-1}$

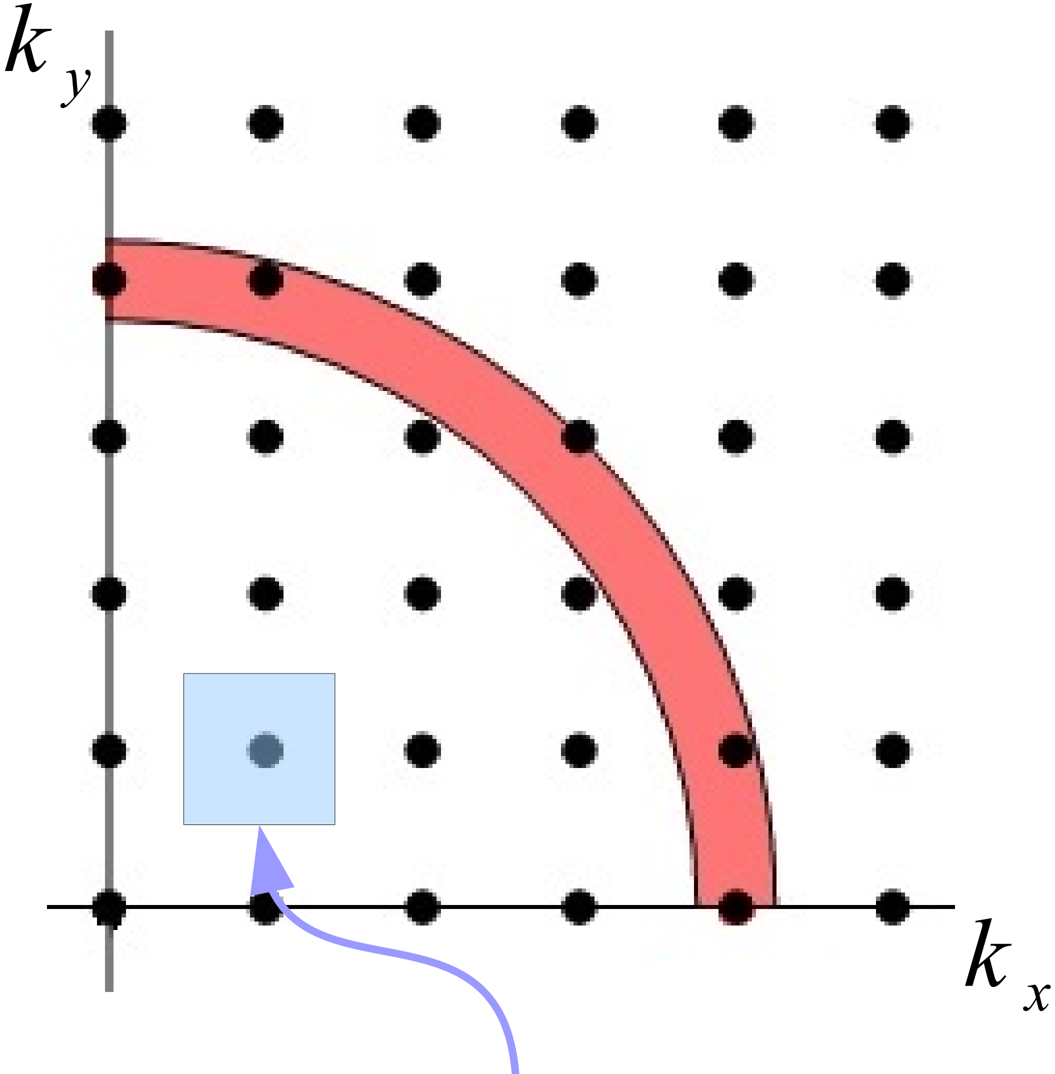
There is no simple pattern of degeneracy

But what happens when the numbers are really large ?

In this case the degeneracy can be visualised geometrically.

How many dots are there inside the annulus for large n_x, n_y (per spin) ?

Each dot = 1 allowed state



1 dot every $(\pi / L)^2$ area

$$k_x = \frac{n_x \pi}{L} \quad : \quad k_x = \frac{n_y \pi}{L}$$

$$k^2 = k_x^2 + k_y^2 = \left(\frac{2mE}{\hbar^2} \right)$$

Area of the annulus

$$= \frac{1}{4} 2 \pi k \delta k = \frac{\pi}{2} \left(\frac{m \delta E}{\hbar^2} \right)$$

$$N(E) \delta E = \frac{L^2}{\pi^2} \frac{\pi}{2} \left(\frac{m \delta E}{\hbar^2} \right)$$

$$\frac{N(E)}{L^2} \delta E = \frac{1}{2} \left(\frac{m}{\pi \hbar^2} \right) \delta E$$

How many dots are there inside the annulus for large n_x, n_y, n_z ?

For a large system, the quantity *N(E)* per unit area, called the density of states plays an important role.

How can one extend the same calculation to *3D* ?

The quandrant of the circle → octant of a sphere and a similar logic will follow

$$\left.\begin{array}{l}\text{3D : per}\\ \text{spin state}\end{array}\right\} \quad \frac{N(E)}{L^3}\,\delta E = \frac{1}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}\,\delta E$$

Notice that the *E(k)* relation plays a role in the expression for *N(E)*. If it is different the result will also be different. The density of states for electrons is not the same as the density of states for photons for example.