

# OBTAINING THE PROBABILITY DENSITY OF FINDING A PARTICLE IN HARMONIC POTENTIAL

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# Introduction

In this section we will solve time independent schrodinger equation by power series method.

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Wave functions  $\psi$  that are physically acceptable must, along with their first derivative  $\frac{d\psi(x)}{dx}$  be define continuous and single valued everywhere, we will see that  $\psi(x)$  must be continuous for the probability density is continuous function of  $x$ .



# Probability Density

According to Born's probability interpretation, the square of the norm of  $\psi(\vec{r}, t)$ .

So  $P(\vec{r}, t) = |\psi(\vec{r}, t)|^2$  represents a position probability density that is the quantity  $|\psi(\vec{r}, t)|^2 d^3r$  represents the probability of finding the particle at time 't' in a volume elements  $d^3r$ .

The total probability of finding the system somewhere in space is equal to 1.

$$\int |\psi(\vec{r}, t)|^2 d^3r = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} |\psi(\vec{r}, t)|^2 dz = 1 \quad (2)$$

A wave function  $\psi(\vec{r}, t)$  satisfying this relation said to be normalized.



# The harmonic oscillator

The mass-spring system where we first introduced unforced harmonic motion. The DE that describes the system is (by Hook's law)

$$F = -kx = m \frac{d^2x}{dt^2} \quad (3)$$



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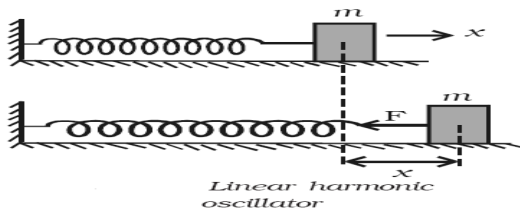


Figure : L.H.O





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$x$ =displacement from equilibrium,  
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and the solution is:

$$x(t) = A\sin(\omega t) + B\cos(\omega t) \quad (5)$$

where

$$\omega = \sqrt{\frac{k}{m}} \quad (6)$$

is the frequency of oscillation.



The potential energy is:

$$V(x) = \frac{1}{2}kx^2; \quad (7)$$

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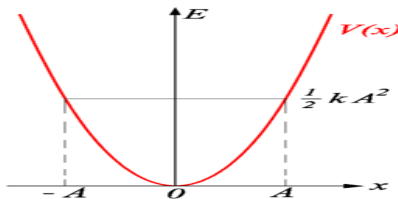
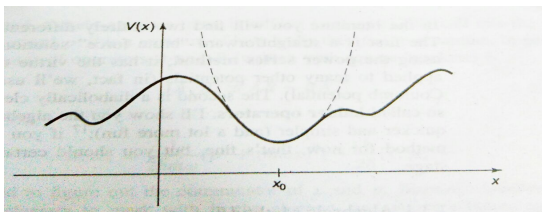


Figure : potential curve



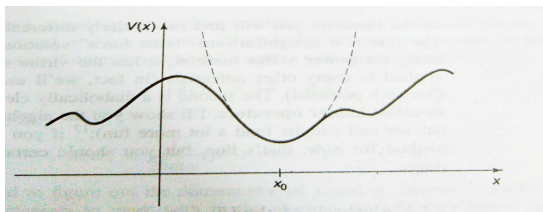
Parabolic approximation to an arbitrary potential, in the neighborhood of a local minimum.



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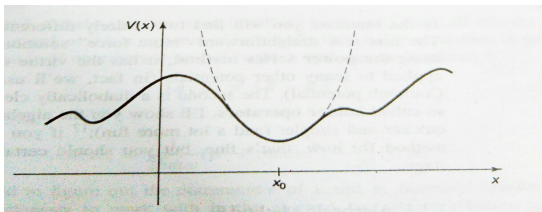
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So,

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put  $V(x)$  in (1) Then Schrodinger equation becomes:-

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Dividing through by the leading term yields:

$$\frac{d^2\psi}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2} x^2\right) \psi = 0 \quad (11)$$



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Thus:

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Dividing through by the leading term gives us:

$$\psi'' + (2\epsilon - y^2)\psi = 0 \quad (17)$$



# Solving the Simplified Equation using Gaussian and Hermite D E:-

The equation now resembles the Gaussian DE  $x'' + (1 - y^2)x = 0$  which has a solution  $e^{-y^2/2}$

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. Therefore the solution to the Schrodinger for the harmonic oscillator is:

$$\psi = \left( \sum_{k=0}^{\infty} c_k y^k \right) e^{-y^2/2}$$



At this point we must consider the boundary conditions for  $\psi$ . We know that  $V(x) = \frac{1}{2}kx^2$ .

Therefore  $\lim_{x \rightarrow \pm\infty} V(x) = \infty$ , which implies that  $\psi(\pm\infty) = 0$ .

This can only be true if the polynomial in the solution above truncates. Recall that in the power series solution to the Hermite DE the following recursion relationship resulted

$$c_{k+2} = \frac{2(k-m)}{(k+2)(k+1)} c_k \quad (23)$$



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then,

$$f(y) = c_0 \left( 1 - \frac{2k}{2!} y^2 + \frac{2^2 k(k-1)}{4!} y^4 - \dots \right) + c_1 \left( y - \frac{2(k-1)}{3!} y^3 + \frac{2^2 (k-1)(k-3)}{5!} y^5 - \dots \right) \dots (24)$$



Since 'k' is a non-negative integer, it is necessary that 'm' is a non-negative integer for the series to truncate. Furthermore, our analysis of the Hermite DE showed that if 'm' is an even integer, it is necessary that  $f'(0) = 0$  for the series to truncate. Similarly, if is odd, it is necessary that  $f(0) = 0$  for truncation to occur. These conditions set up the Hermite polynomials

$$H_m(y) = \sum_{k=0}^{\lceil \frac{m}{2} \rceil} \frac{(-1)^k m!}{k!(m-2k)!} (2x)^{m-2k} \quad (25)$$

where  $\lceil \frac{m}{2} \rceil$  is greatest integer



thus a given value of 'm' :

$$\psi_m = c_m H_m(y) e^{-y^2/2} \quad (26)$$

Where  $c_m$  is a constant. We now back substitute, recalling that previously we let  $y = \sqrt{\frac{m\omega}{\hbar}} x$





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Therefore:

$$\psi_m = c_m H_m\left(\sqrt{\frac{m\omega}{\hbar}} x\right) e^{-\frac{m\omega}{2\hbar} x^2} \quad (27)$$

The wave function  $\psi$  is indexed indicating that the wave forms are different for different values of m.



### Determining the Constant $c_m$ :-

The constant  $c_m$  is determined by normalizing  $\psi$ ,  
i.e.

$$|\psi_m(x)|^2 = \int_{-\infty}^{+\infty} \psi_m^2(x) dx = 1 \quad (28)$$

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



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The orthogonality of Hermite polynomials, we know that:

$$\int_{-\infty}^{+\infty} H_m^2(u) e^{-u^2} du = 2^m m! \sqrt{\pi}$$

and therefore,

$$c_m^2 2^m m! \sqrt{\pi} = \sqrt{\frac{m\omega}{\hbar}}$$



$$\Rightarrow c_m = \left( \frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{2^m m!}}$$

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$$\psi_m = \left( \frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \frac{1}{\sqrt{2^m m!}} H_m \left( \sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{m\omega}{2\hbar} x^2} \quad (30)$$





and,

$$|\psi_m|^2 = \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{2}} \frac{1}{2^m m!} |H_m(\alpha x)|^2 e^{(-\frac{\alpha^2}{2} x^2)^2} \quad (32)$$



# Analysis of wave function and probability density:

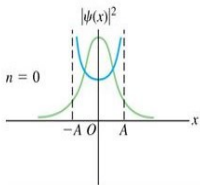
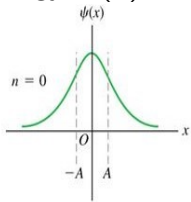
Each wave function is associated with a hermite polynomial  $H_m(x)$ . Given table is first 8 wave functions  $\psi_m$  corresponding hermite polynomials. And  $|\psi_m|^2$  is corresponding probability density of finding a particle in harmonic potential.

$m$	$E_m$	$H_m(x)$	$\Psi_m$
0	$\frac{1}{2} \hbar \omega$	1	$\left(\frac{\alpha}{\pi}\right)^{1/4} H_0(\alpha x) e^{-\frac{\alpha^2 x^2}{2}}$
1	$\frac{3}{2} \hbar \omega$	$2x$	$\left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} H_1(\alpha x) e^{-\frac{\alpha^2 x^2}{2}}$
2	$\frac{5}{2} \hbar \omega$	$4x^2 - 2$	$\left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{2\sqrt{2}} H_2(\alpha x) e^{-\frac{\alpha^2 x^2}{2}}$
3	$\frac{7}{2} \hbar \omega$	$8x^3 - 12x$	$\left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{4\sqrt{3}} H_3(\alpha x) e^{-\frac{\alpha^2 x^2}{2}}$
4	$\frac{9}{2} \hbar \omega$	$16x^4 - 48x^2 + 12$	$\left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{8\sqrt{6}} H_4(\alpha x) e^{-\frac{\alpha^2 x^2}{2}}$
5	$\frac{11}{2} \hbar \omega$	$32x^5 - 160x^3 + 120x$	$\left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{16\sqrt{15}} H_5(\alpha x) e^{-\frac{\alpha^2 x^2}{2}}$
6	$\frac{13}{2} \hbar \omega$	$64x^6 - 480x^4 + 720x^2 - 120$	$\left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{96\sqrt{5}} H_6(\alpha x) e^{-\frac{\alpha^2 x^2}{2}}$
7	$\frac{15}{2} \hbar \omega$	$128x^7 - 1344x^5 + 3360x^3 - 1680x$	$\left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{96\sqrt{70}} H_7(\alpha x) e^{-\frac{\alpha^2 x^2}{2}}$

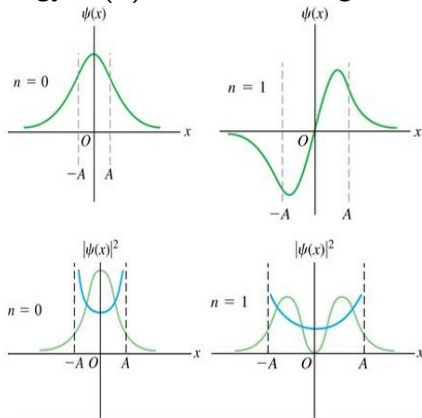
table of hermite polynomials and wave functions



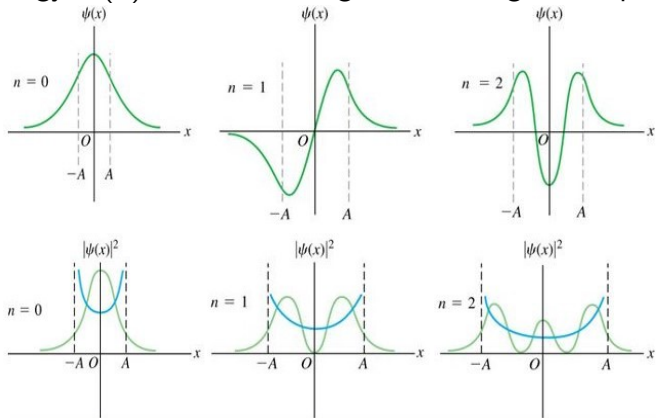
The wave functions and probability distribution functions are plotted below. Each plot has been shifted upward so that it rests on its corresponding energy level. The parabola represents the potential energy  $V(x)$  of the restoring force for a given displacement



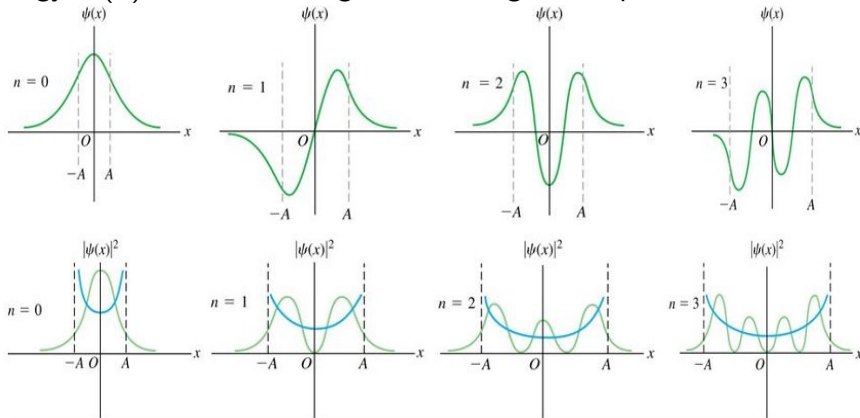
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graphs of wave functions and probability distributions





# References

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*Thank you*

