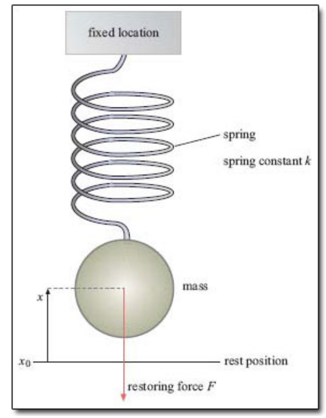
The Quantum Harmonic Oscillator



Classical Analysis

Recall the mass-spring system where we first introduced unforced harmonic motion. The DE that describes the system is:

$$M\frac{d^2x}{dt^2} + Kx = 0$$

where:

$x =$ displacement from equilibrium,
$M =$ mass of the object,
$K =$ spring constant.

> Note that throughout this discussion the variables m and k will also be used where:
> m = index for an m^{th}-order Hermite polynomial,
> k = index for a power series summation.

The solution of this system is:

$$x = c_1 sin\left(\sqrt{\frac{K}{M}}t\right) + c_2 sin\left(\sqrt{\frac{K}{M}}t\right).$$

We define ω to be the natural frequency of the system such that:

$\omega = \sqrt{\frac{K}{M}} x = c_1 sin(\omega t) + c_2 sin(\omega t)$Note this means:

$$K = \omega^2 M$$

We will use this result shortly.

Quantum Analysis

Thus far we have described the harmonic oscillator in classical sense. At this point we use the Schrödinger equation to describe the system in quantum sense. Recall:

$$-\frac{\hbar^2}{2M}\frac{d^2\psi(\mathrm{x})}{dx^2}+V(x)\psi(\mathrm{x})=E\psi(\mathrm{x}),$$

where,

$\hbar$	$h/2\pi$ (reduced Plank's constant)
h	Plank's constant (describes size of quanta in quantum mechanics)
M	mass of particle
$\psi(\mathrm{x})$	time independent wave function
$V(x)$	potential energy of particle
E	total energy of particle

We model the force on the particle using the classical idea of a spring system; hence the potential energy $V(x)$ is due to the spring's restoring force $F=-Kx$ and is given by:

$$V(x)=-\int F dx=-\int -Kx dx=\frac{1}{2}Kx^2,$$

Since $K=M\omega^2$, potential energy is rewritten as:

$$V(x)=\frac{1}{2}M\omega^2x^2.$$

The Schrödinger equation becomes:

$$-\frac{\hbar^2}{2M}\frac{d^2\psi}{dx^2}+\frac{1}{2}M\omega^2x^2\psi=E\psi \longrightarrow \frac{\hbar^2}{2M}\frac{d^2\psi}{dx^2}+\left(E-\frac{1}{2}M\omega^2x^2\right)\psi=0.$$

Dividing through by the leading term yields:

$$\frac{d^2\psi}{dx^2}+\left(\frac{2ME}{\hbar^2}-\frac{M^2\omega^2}{\hbar^2}x^2\right)\psi=0$$

Using Substitutions to Simplify the Equation

First let:

$$\epsilon=\frac{E}{\hbar\omega}\longrightarrow E=\hbar\omega\epsilon,$$

The Schrödinger equation becomes:

$$\frac{d^2\psi}{dx^2} + \left(\frac{2M\omega\epsilon}{\hbar} - \frac{M^2\omega^2}{\hbar^2}x^2\right)\psi = 0$$

Now let:

$$y = \sqrt{\frac{M\omega}{\hbar}}x \rightarrow x = \sqrt{\frac{\hbar}{M\omega}}y.$$

Thus:

$$\frac{d\psi}{dx} = \frac{d\psi}{dy}\frac{dy}{dx} = \sqrt{\frac{M\omega}{\hbar}}\frac{d\psi}{dy} \quad \left(\text{note from above}\,\frac{dy}{dx} = \sqrt{\frac{M\omega}{\hbar}}\right),$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dy}\left(\sqrt{\frac{M\omega}{\hbar}}\frac{d\psi}{dy}\right) = \sqrt{\frac{M\omega}{\hbar}}\frac{d}{dy}\left(\frac{d\psi}{dy}\right) = \sqrt{\frac{M\omega}{\hbar}}\frac{d^2\psi}{dy^2}\frac{dy}{dx} = \frac{M\omega}{\hbar}\frac{d^2\psi}{dy^2},$$

yielding:

$$\frac{M\omega}{\hbar}\psi'' + \left(\frac{2M\omega\epsilon}{\hbar} - \frac{M\omega}{\hbar}y^2\right)\psi = 0.$$

Dividing through by the leading term gives us:

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

Solving the Simplified Equation using Gaussian and Hermite Differential Equations

The equation now resembles the Gaussian DE $x'' + (1 - y^2)x = 0$ which has a solution $e^{-y^2/2}$. One plausible guess for the solution to the above equation is $\boldsymbol{\psi = f(y)e^{-y^2/2}}$. Thus:

$$\psi' = f'(y)e^{-y^2/2} - yf(y)e^{-y^2/2} = \left(f'(y) - yf(y)\right)e^{-y^2/2}$$
$$\psi'' = f''(y)e^{-y^2/2} - yf'(y)e^{-y^2/2} - f(y)e^{-y^2/2} - yf'(y)e^{-y^2/2} + y^2f(y)e^{-y^2/2} \rightarrow$$

$$\boldsymbol{\psi'' = \left(f''(y) - 2yf'(y) - f(y) + y^2f(y)\right)e^{-y^2/2}}$$

Plugging this into the Schrödinger equation yields:

$$\left(\boldsymbol{f''(y) - 2yf'(y) - f(y) + y^2 f(y)}\right)\boldsymbol{e^{-y^2/2}} + (2\epsilon - y^2)\boldsymbol{f(y)e^{-y^2/2}} = 0,$$

which simplifies to:

$$\left(f''(y) - 2yf'(y) + (2\epsilon - 1)f(y)\right)e^{-y^2/2} = 0.$$

Dividing out the exponential yields:

$$f''(y) - 2yf'(y) + (2\epsilon - 1)f(y) = 0.$$

Setting $2\epsilon - 1 = 2m$ generates:

$$f''(y) - 2yf'(y) + 2mf(y) = 0,$$

which is the Hermite differential equation. The solution of the DE is represented as a power series $\sum_{k=0}^{\infty} c_k y^k$. Therefore the solution to the Schrödinger for the harmonic oscillator is:

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

At this point we must consider the boundary conditions for ψ. We know that $V(x) = \frac{1}{2}m\omega^2 x^2$. Therefore $\lim_{x\to\pm\infty} V(x) = \infty$, 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:

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

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 *y'(0)=0* for the series to truncate. Similarly, if m is odd, it is necessary that *y(0)=0* for truncation to occur. These conditions set up the Hermite polynomials $H_m(y)$, thus a given value of m:

$$\boldsymbol{\psi_{\mathrm{m}} = c_m H_m(y) e^{-y^2/2}},$$

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

Therefore:

$$\boldsymbol{\psi_{\mathrm{m}} = c_m H_m\left(\sqrt{\frac{M\omega}{\hbar}}x\right)e^{-\frac{M\omega}{2\hbar}x^2}}.$$

The wave function $\boldsymbol{\psi_{\mathrm{m}}}$ is indexed indicating that the wave forms are different for different values of m.

<u>Determining the Constant</u>

The constant c_m is determined by normalizing Ψ, i.e.:

$$|\psi_{\mathrm{m}}(\mathrm{x})|^2 = \int_{-\infty}^{\infty}[\psi_{\mathrm{m}}(\mathrm{x})]^2 \mathrm{dx} = 1.$$

This is necessarily true since $|\Psi_{\mathrm{m}}(\mathrm{x})|^2$ is a probability distribution function . Therefore:

$$c_m^2\int_{-\infty}^{\infty} H_m^2\left(\sqrt{\frac{M\omega}{\hbar}}x\right)e^{-\frac{M\omega}{\hbar}x^2}dx = 1 \qquad \left(\text{Note: }\left(e^{-\frac{M\omega}{2\hbar}x^2}\right)^2 = e^{-\frac{M\omega}{\hbar}x^2}\right)$$

Using substitutions techniques from integral calculus let:

$$u = \sqrt{\frac{M\omega}{\hbar}}x \longrightarrow \mathrm{du} = \sqrt{\frac{M\omega}{\hbar}}dx \longrightarrow \mathrm{dx} = \sqrt{\frac{\hbar}{M\omega}}\mathrm{d}u,$$

thus:

$$c_m^2\sqrt{\frac{\hbar}{M\omega}}\int_{-\infty}^{\infty}H_m^2(u)e^{-u^2}du = 1 \longrightarrow c_m^2\int_{-\infty}^{\infty}H_m^2(u)e^{-u^2}du = \sqrt{\frac{M\omega}{\hbar}}.$$

From our previous discussion of 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:

$$c_m^2 2^m m!\sqrt{\pi} = \sqrt{\frac{M\omega}{\hbar}} \longrightarrow \mathrm{c_m} = \left(\frac{M\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^m m!}},$$

which gives us our final solution:

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

By letting $\alpha = \sqrt{\frac{M\omega}{\hbar}}$, we can rewrite ψ_m:

$$\psi_m = \left(\frac{\alpha^2}{\pi}\right)^{1/4} \frac{1}{\sqrt{2^m m!}} H_m(\alpha x) e^{-\frac{\alpha^2 x^2}{2}}$$

Quantization of Energy

Recall that in the course of this derivation, the following substitutions were made:

$$E = \hbar\omega\epsilon,$$

and:

$$2\epsilon - 1 = 2m \longrightarrow \epsilon = m + \frac{1}{2},$$

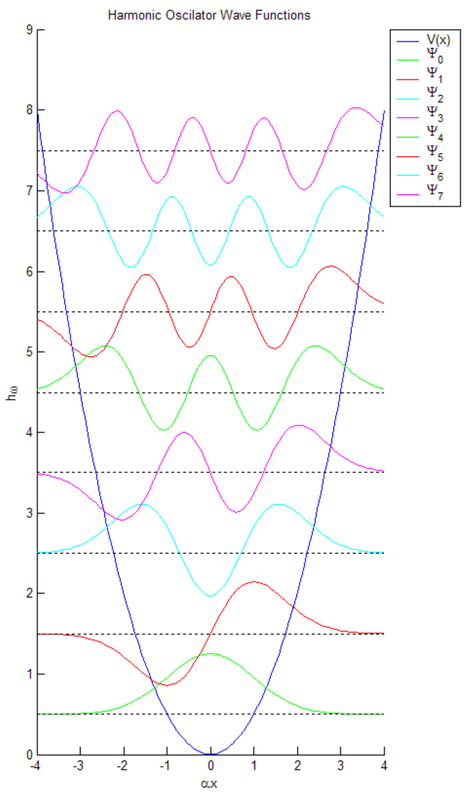
therefore:

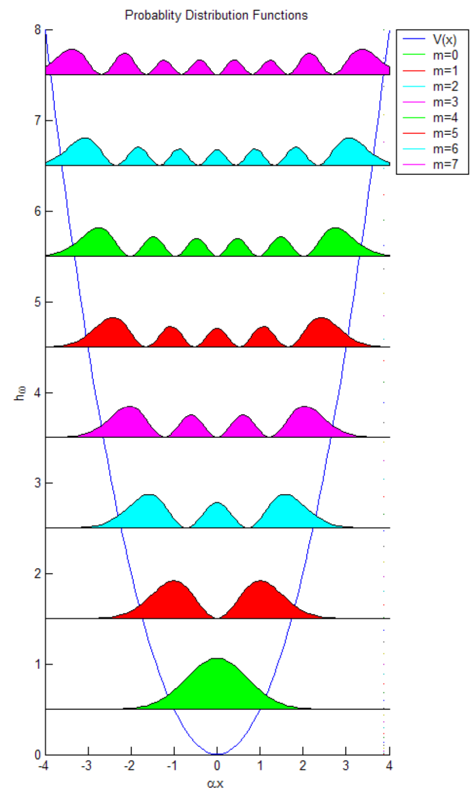
$$\boxed{E_m = \left(m + \frac{1}{2}\right)\hbar\omega}$$

Since m is a non-negative integer, then E_m can only take on discrete values, i.e E_m is quantized. Each energy level is associated with a specific wave function ψ. Below is a table of the first 8 energy levels and corresponding wave functions.

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

The wave functions and probablilty distribution functions are ploted 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.





Example: If a particle exists in the second energy level. What is the probability that the particle is found in the interval $1 \leq \alpha x \leq 2 \rightarrow 1/\alpha \leq x \leq 2/\alpha$.

First determine what ψ_2 actually looks like:

$$\psi_2 = \left(\frac{\alpha^2}{\pi}\right)^{1/4} \frac{1}{2\sqrt{2}} H_2(\alpha x) e^{-\frac{\alpha^2 x^2}{2}} \rightarrow$$

$$\psi_2 = \left(\frac{\alpha^2}{\pi}\right)^{1/4} \frac{1}{2\sqrt{2}} (4x^2 - 2) e^{-\frac{\alpha^2 x^2}{2}}$$

Recall that $\Pr(1/\alpha \leq x \leq 2/\alpha) = \int_{1/\alpha}^{2/\alpha} |\psi_2|^2 dx$. This equals:

$$\int_{1/\alpha}^{2/\alpha}\left[\left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}}\frac{1}{2\sqrt{2}}(4(\alpha x)^2-2)e^{-\frac{\alpha^2x^2}{2}}\right]^2 dx$$

Let $u=\alpha x\rightarrow du=\alpha dx\rightarrow dx=\frac{du}{\alpha}\rightarrow$

$$\int_{1}^{2}\left[\left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}}\frac{1}{2\sqrt{2}}(4u^2-2)e^{-\frac{u^2}{2}}\right]^2 \frac{du}{\alpha}$$

$$=\int_1^2\frac{\alpha}{8\sqrt{\pi}}(4u^2-2)^2e^{-u^2}\frac{du}{\alpha}$$

$$=\frac{1}{8\sqrt{\pi}}\int_1^2(4u^2-2)^2e^{-u^2}du=$$

<u>Homework</u>: What is the probability that the particle is found in the interval $2\leq\alpha x\leq 3$ for a particle in the $m=3$ energy level?