

The Simple Harmonic Oscillator I

Outline:

□ Why the SHO?

□ Solving it in the traditional method

Why the harmonic oscillator?

The harmonic oscillator is perhaps the most important problem in all of quantum physics. QFT, which is the basis of almost all of the major breakthroughs of 20th century physics, relies on the intuition gleaned from the harmonic oscillator.

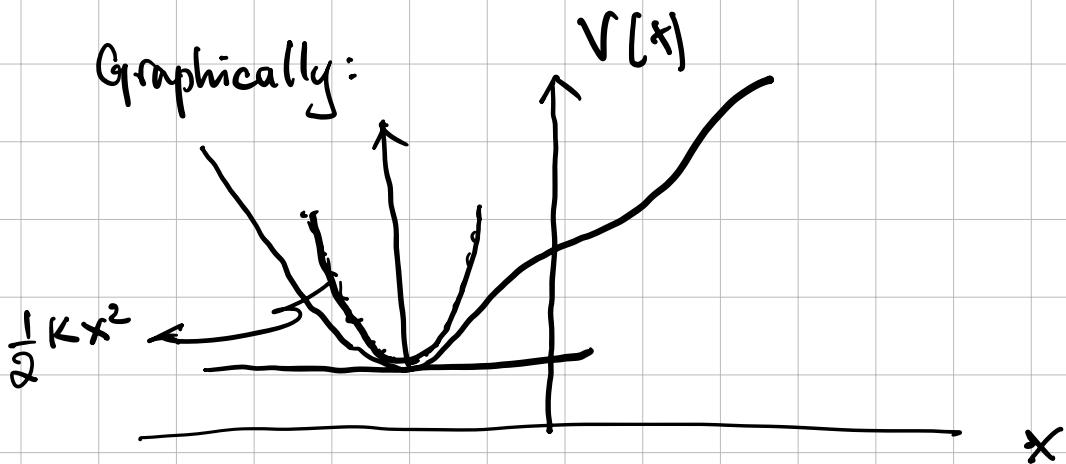
For bound systems the expansion of the potential around its minima, x_0 , will be given by:

$$V(x-x_0) = V(x_0) + (x-x_0)^2 \left. \frac{d^2 V}{dx^2} \right|_{x=x_0} + \dots$$

The $V'(x_0) = 0$ by definition.

So by a suitable redefinition of the classical zero-point energy $V(x_0)$ we can write V as:

$$V(x) = \frac{1}{2} Kx^2 + \dots \text{ for some } K > 0.$$



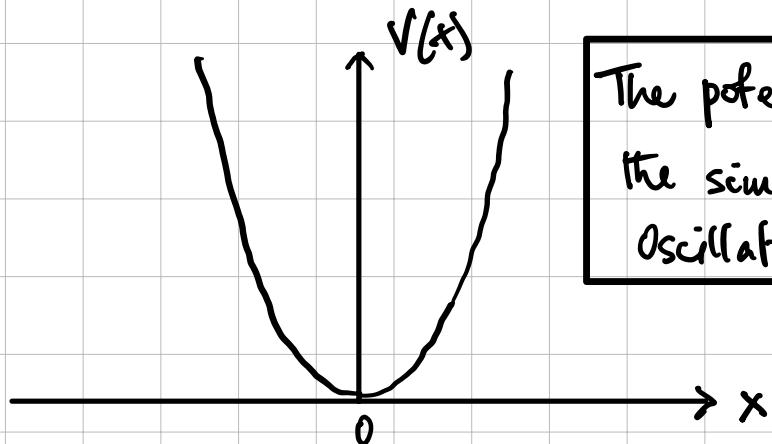
Thus we see that for small oscillations we can approximate the dynamics of a bounded system by the 'harmonic form' $\frac{1}{2} Kx^2$.

Ex: Small atomic oscillations in solids.

The Hamiltonian:

The Hamiltonian of the SHO is

$$H = \frac{p^2}{2m} + \frac{1}{2} Kx^2$$



Classical solution:

$$x = a \cos(\omega t + \phi)$$

where $\omega = \sqrt{k/m}$ [verify.]

Total energy:

$$E = \frac{1}{2} K a^2 = \frac{1}{2} m \omega^2 a^2$$

Quantum mechanically we have $H\psi = E\psi$ which becomes:

Time independent Schrödinger equation:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} \left(E - \frac{1}{2} kx^2 \right) \psi = 0$$

For convenience let us choose $E_0 \equiv \frac{1}{2}\hbar\omega$ to be the unit of energy.

$$E = \lambda \frac{1}{2}\hbar\omega$$

and we use the classical amplitude of oscillations, a for the energy $\frac{1}{2}\hbar\omega$, to be our unit of distance:

$$a = \sqrt{\frac{\hbar}{m\omega}}$$

Then defining $x = x'a$ we get after a couple of lines of algebra:

$$\frac{m\omega}{\hbar} \left(\frac{d^2\psi}{dx'^2} + (1-x'^2)\psi \right) = 0$$

Relabelling $x' \rightarrow x$ we get

$$\frac{d^2\psi}{dx^2} + (\lambda - x^2)\psi = 0$$

Rescaled KE $\sim -\frac{d^2\psi}{dx^2} + x^2\psi = \lambda\psi$ Rescaled potential energy
Rescaled energy eigenvalue

This is an eigenvalue equation as it has the form

$$\hat{O}\psi = \lambda\psi$$

\hat{O}
operator.

Positivity of the energy:

It is easy to show that the energy eigenvalues of the harmonic oscillator are positive. For this let's revert back to the original variables:

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

Recall that for Hermitian operators \hat{O} we have

$$(\psi, \hat{O}\phi) = (\hat{O}\psi, \phi)$$

This means that for any state ψ :

$$\begin{aligned}\langle H \rangle_{\psi} &= (\psi, \hat{H} \psi) = (\psi, \frac{\hat{p}^2}{2m} \psi) + \frac{1}{2} K (\psi, \hat{x}^2 \psi) \\ &= \frac{1}{2m} (\hat{p} \psi, \hat{p} \psi) + \frac{1}{2} K (\hat{x} \psi, \hat{x} \psi)\end{aligned}$$

[We have used $\hat{\cdot}$'s to emphasize that p & x are operators.]

Let $\phi = \hat{p} \psi$

and $x = \hat{x} \psi$

then we have

$$\langle H \rangle_{\psi} = \frac{1}{2m} (\phi, \phi) + \frac{1}{2} K (x, x)$$

Since $(\phi, \phi) \geq 0$ and $(x, x) \geq 0$ we get:

$$\langle H \rangle_{\psi} \geq 0 \text{ for all } \psi.$$

If we choose ψ to be an energy eigenstate

$$H \psi = E \psi$$

$$\Rightarrow \langle H \rangle \geq 0 \Rightarrow E \geq 0.$$

Thus we see that the energy eigenvalues are positive

Semi-definite

Solving the differential equation:

Our SE has the form:

$$\psi'' + (\lambda - x^2) \psi = 0. \quad (†)$$

Since this is a bounded potential we expect $\psi \rightarrow 0$ as $|x| \rightarrow \infty$. So let us try to solve (†) asymptotically.

For large $|x|$ we can ignore the λ term and our equation becomes :

$$\psi'' \sim x^2 \psi$$

It is easy to verify that $\psi = C x^n e^{\pm \frac{1}{2} x^2}$ are both solutions to the asymptotic equation. (We are taking $e^{+\frac{1}{2} x^2}$ even though it doesn't match our boundary condition because it is still a formal solution.)

$$\psi' = C n x^{n-1} e^{\pm \frac{1}{2} x^2} \pm C x^{n+1} e^{\pm \frac{1}{2} x^2}$$

$$\psi'' = C n(n-1) x^{n-2} e^{\pm \frac{1}{2} x^2}$$

$$\pm C n x^n e^{\pm \frac{1}{2} x^2}$$

$$\begin{aligned} & \pm C(n+1)x^n e^{\pm \frac{1}{2}x^2} \\ & + Cx^{n+2} e^{\pm \frac{1}{2}x^2} \\ \psi'' = & Cx^{n+2} e^{\pm \frac{1}{2}x^2}. \end{aligned}$$

$$\left\{ 1 \pm \frac{(2n+1)}{x^2} + \frac{n(n-1)}{x^4} \right\}$$

In the limit $|x| \rightarrow \infty$ we thus get

$$\begin{aligned} \psi'' &= x^2 \left(Cx^n e^{\pm \frac{1}{2}x^2} \right) \\ &= x^2 \psi \end{aligned}$$

So we expect our exact solution to
be something of the form:

$$\psi(x) = \phi(x) e^{-\frac{1}{2}x^2}$$

$$\psi'' + (\lambda - x^2)\psi = 0. \quad (†)$$

Plugging this into (†) we get

$$\psi' = \phi' e^{-\frac{1}{2}x^2} - \phi x e^{-\frac{1}{2}x^2}$$

$$\psi'' = \phi'' e^{-\frac{1}{2}x^2} - \phi' x e^{-\frac{1}{2}x^2}$$

$$- \phi' x e^{-\frac{1}{2}x^2}$$

$$- \phi e^{-\frac{1}{2}x^2} + \phi x^2 e^{-\frac{1}{2}x^2}$$

$$\phi'' - x\phi' - \phi'x - \phi + \phi x^2$$

$$+ (\lambda - x^2)\phi = 0$$

$$\phi'' - 2\phi'x + (\lambda - x^2 - 1 + x^2)\phi = 0$$

$$\boxed{\phi'' - 2x\phi' + (\lambda - 1)\phi = 0}$$

Series solution:

$$\phi(x) = \sum_{n=0}^{\infty} a_n x^n$$

$$\begin{aligned}\phi'(x) &= \sum_{n=0}^{\infty} n a_n x^{n-1} \\ &= \sum_{n=0}^{\infty} n a_n x^{n-1}\end{aligned}$$

$$\begin{aligned}\phi''(x) &= \sum_{n=1}^{\infty} n(n-1) a_n x^{n-2} \\ &= \sum_{n=0}^{\infty} n(n-1) a_n x^{n-2}\end{aligned}$$

Thus we get :

$$\sum_{n=0}^{\infty} [n(n-1) a_n x^{n-2} - 2n a_n x^n + (\lambda-1) a_n x^n] = 0$$

$$\text{or } \sum_{n=0}^{\infty} [n(n-1) a_n x^{n-2} - (2n - (\lambda-1)) a_n x^n] = 0$$

We equate coefficients of equal powers of x
to each other :

$$\underline{x^{-2}}: 0 \cdot (-1) a_0 = 0$$

$$\underline{x^{-1}}: 1 \cdot (0) \cdot a_1 = 0$$

$$\underline{x^0}: 2 \cdot 1 \cdot a_2 - [2 \cdot 0 - (\lambda-1)] a_0 = 0$$

$$\underline{x^n}: (n+2)(n+1) a_{n+2} = [2n - (\lambda-1)] a_n$$

$$a_{n+2} = \frac{2n - (\lambda - 1)}{(n+2)(n+1)} a_n$$

Recursion Relation

Note that the values a_0 and a_1 are not fixed. So we are free to choose:

$a_0 = 0$ then we get the solution:

$$1) \quad \phi_1 = a_1 x + a_3 x^3 + a_5 x^5 + \dots \quad \text{odd function}$$

On the other hand if we choose $a_1 = 0$ we get

$$2) \quad \phi_0 = a_0 + a_2 x^2 + a_4 x^4 + \dots \quad \text{even function}$$

It should be clear that $\phi_0(x)$ and $\phi_1(x)$ are linearly independent solutions due to their different parities.

Quantization of energy

The series solutions as we have derived them cannot continue for indefinitely. To see this let us compare

two consecutive terms:

$$\frac{a_{n+2} x^{n+2}}{a_n x^n} = \frac{2n - (\lambda - 1)}{(n+1)(n+2)} x^2$$

For large values of n we see that this ratio goes over to $\frac{2}{n} x^2$. This is a convergent series but it has the same asymptotic behaviour as

$$e^{x^2} = \sum_{n=0}^{\infty} \frac{(x^2)^n}{n!} = \sum_{\substack{n=0 \\ n \text{ even}}}^{\infty} \frac{x^n}{(n/2)!}.$$

Thus the functions ϕ_0 and ϕ_1 behave like e^{x^2} when x is large. Thus they are not bounded and are not suitable to be used as wavefunction.

Another thing to note that this analysis does not put any constraints on the value of λ but we know that λ cannot be negative.

We are released from both of these problems if at some point the series in ϕ_0 and ϕ_1 terminate. The only way this can happen is when for some value of n we get:

$$2n - (\lambda - 1) = 0 \Rightarrow \lambda - 1 = 2n$$

$$\lambda_n = 2n + 1$$

This implies that our energy is quantized:

$$E_n = \frac{1}{2} \hbar \omega \lambda_n$$

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega$$

This is perhaps the most famous equation in quantum mechanics. Several comments are in order:

1. The quantization of energy is related to the requirement that the particle be bounded. So quantization of energy is an essential feature of bound system, i.e. systems whose total energy is negative. (E.g. the solar system.)
2. For large n we get $E_n \sim n \hbar \omega$. This is precisely the Planck hypothesis. So this agrees with our assumption that the atoms of the wall of a black body cavity are oscillators with quantized energy levels.

3 The zero point energy or the vacuum energy is $E_0 = \frac{1}{2}\hbar\omega$ for $n=0$ is non-zero. So the lowest energy state (known as the vacuum state) is not a zero energy state. We shall see that this has to do with the uncertainty principle.

The Hermite Polynomials

The functions ϕ_0 and ϕ_1 have very specific structure. These are polynomials due to the quantization of energy. These polynomials are called the Hermite polynomials and are denoted by $H_n(x)$. Since the values of a_0 and a_1 are arbitrary we can fix them by demanding that highest power of x in $H_n(x)$ has the coefficient 2^n . Then the first few Hermite polynomials are:

$$H_0(x) = 1, \quad H_1(x) = 2x, \quad H_2(x) = 4x^2 - 2$$

$$H_3(x) = 8x^3 - 12x, \dots$$

So the wavefunctions are given by:

$$\psi_n(x) = C_n H_n(x) e^{-x^2/2}$$

where C_n s are normalization constants.

Properties of Hermite Polynomials

The Hermite differential equation is

$$H_n'' - 2xH_n' + 2nH_n = 0 \quad \text{for } n \in \mathbb{Z}_+$$

The Hermite polynomials are solutions. Just as the functions e^{ikx} provide a complete basis for expressing wavefunctions on a Hilbert space, the Hermite polynomials also provide a complete basis of functions. However, this aspect of H_n shall not be explored here.

It is not very hard to prove the following recursion relations for H_n s: (Show)

1. $H_n' = 2n H_{n+1}$

2. $H_{n+1} - 2xH_n + 2nH_{n-1} = 0$

3. $H_{n+1} = 2xH_n - H'$

Given $H_0 = 1$, one can use no. 3 of the above relations to derive higher H_n s.

The Generating Function

There is a very elegant way to encode all the Hermites in one master function. This function is called the generating function:

$$g(x, h) = \sum_{n=0}^{\infty} H_n(x) \frac{h^n}{n!}$$

So, if we could find this function g then we could extract any $H_n(x)$ we needed by taking the derivative of g w.r.t. h n times and then setting $h=0$.

Using the recursion relations above it is easy to derive a differential eqn for g :

$$\frac{dg}{dh} = (2x - 2h)g$$

which is easily integrated to show that

$$g(x, h) = C(x) e^{2xh - h^2}$$

The integration 'constant' is fixed by the boundary

$$\text{condition } g(x, 0) = C(x) = H_0(x) = 1$$

$$\text{And so } g(x, h) = e^{2xh - h^2}.$$

$$\text{Thus we get } H_n(x) = \left. \frac{\partial^n}{\partial h^n} e^{2xh - h^2} \right|_{h=0}$$

This can be reexpressed as

$$H_n(x) = (-)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}$$

The generating functional approach is very powerful and can be used to show that :

$$C_n = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}}$$

$$\text{and } \psi_n = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} e^{-x^2/2} H_n(x)$$

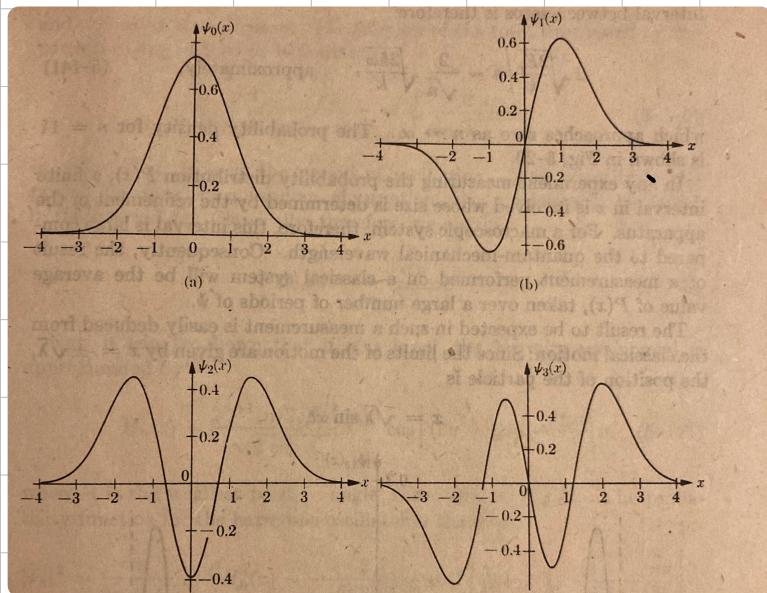
The wave functions are orthonormal:

$$\int_{-\infty}^{+\infty} dx \psi_m^*(x) \psi_n(x) = \delta_{mn}$$

Note that because $e^{-x^2/2}$ is an even function and the Hermites are even or odd functions our resulting wave functions $\psi_n(x)$ are either even

or odd as we have discussed in a previous lecture about systems with symmetric potentials

The first few wave-functions are:



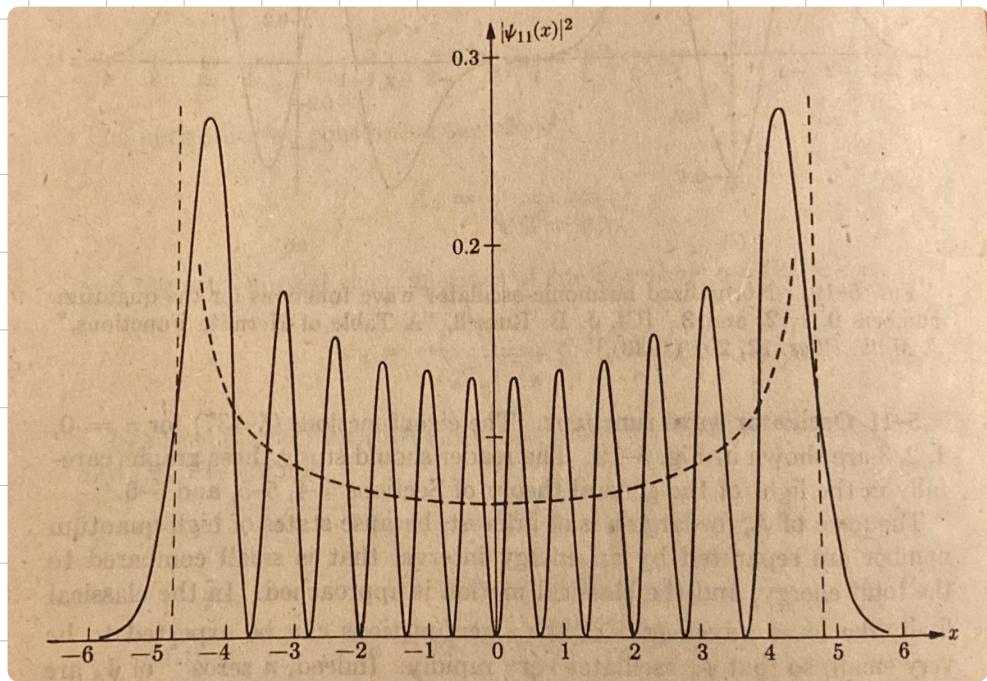
The 'classical' limit:

If we compare the quantum harmonic oscillator with its classical counterpart we may wonder how can the two be connected. This is a subtle and deep question which is related to the theory of 'coherent states' (something we won't cover in this course).

But we can do some crude comparisons. E.g. if

we look at the ground state wavefunction we see that the most probable position of the particle is $x=0$. But on the other hand for a classical oscillator it spends 'more' time at the extreme end of its oscillations than in the middle so we expect the opposite probability distribution for the classical oscillator.

The way out of this is to invoke the correspondence principle and argue that the quantum case should agree with the classical case only when the energy of the quantum oscillator is large.



It turns out that we don't have to go that high up to see a qualitative agreement as the following graph of Ψ_{11} and the classical probability distribution shows. The classical distribution is given by the broken lines.