Quantum Harmonic Oscillator

The classical harmonic oscillator has energy

$$E_{osc.}=\frac{p^2}{2m}+\frac12m\omega^2x^2\ ,\quad\omega=\sqrt{\frac{k}{m}}$$

When the harmonic oscillator was first studied by physicist under the lens of the quantum realm, there was the need to construct a viable Hamiltonian.

$$H_{osc.}=\frac{\hat p^2}{2m}+\frac12m\omega^2\hat x^2\ ,\quad\left[\hat x,\hat p\right]=i\hbar$$

It's a quantum mechanical system inspire from classical mechanics in the simplest and purest way. Studying it one can see that the oscillator has specific allowed values of amplitude and energy.

Results from such a study can be used almost anywhere. Any system with an equilibrium point has an oscillator-like potential in the neighbouring region, at least in approximation. Meaning that all systems in equilibrium can be approximated up to a degree with a harmonic oscillator.

Just like the infinite well, the potential blows up to infinity, and as such all allowed states of a particle are **bound states**.

The eigenvalue equation is: $$\hat H\psi_n(x)=E_n\psi_n(x)$$

There are two ways to solve the eigenvalue problem. The first is a brute force solution of the differential equation, and in the process finding out the quantization of energy directly from the form of the equation. The second way is to solve it algebraically by defining the appropriate creation and annihilation operators, which move the system to the next or previous energy state respectively.

Natural Units

The complete equation is:

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac12m\omega^2x^2\psi(x)=E\psi(x)} \tag{1}$$

The first obstacle we find when we try to solve it is all those quantities with their respective units. There are two practical ways to get rid of them. The first one is the use of **natural units**, $\hbar=m=\omega=1$, and then some kind of multiplication between them and the results in order to recreate the proper physical units. Then the problem reduces to the form below:

$$\psi''(x)+\left(2E-x^2\right)\psi(x)=0 \tag{2}$$

The *problem* with this approach when first learning about the quantum harmonic oscillator is that you kind have to already know before what type of result you expect and what unit reconstruction to do, or blindly trust your textbook, ending up in not understanding what you're doing (*that's what happened to me at least*).

The second approach is starting by demanding the use of a dimensionless variable, and then find

what combination of constants makes x dimensionless.

Using a Dimensionless Variable

We write the variable x as $x=\alpha u$, where u is dimensionless and α has units of length. The kinetic energy part of the equation can be now written as:

$$ -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} =-
\frac{\hbar^2}{2m}\frac{d^2\psi}{\left(d\left(\alpha u\right)\right)^2}
=\frac{\hbar^2}{m\alpha^2}\cdot\left(-\frac12\frac{d^2\psi}{du^2}\right) $$

Similarly, the potential energy part is:

$$ \frac12m\omega^2x^2\psi(x) =\frac12m\omega^2\left(\alpha u\right)^2\psi(u)
=m\omega^2\alpha^2\cdot\left(\frac12u^2\psi(u)\right) $$

On the other side of the equation we only have $E\psi(u)$, and hence we have two ways to construct the energy from the constants.

$$ E=\frac{\hbar^2}{m\alpha^2}=m\omega^2\alpha^2 \Leftrightarrow
\boxed{\alpha^2=\frac{\hbar}{m\omega}} $$

Putting this back to equation (1) we have: $$- \frac12\frac{\hbar^2}{ma^2}\frac{d^2\psi}{du^2}
+\frac12m\omega^2a^2u^2\psi(u) =E\psi(u) $$ $$ -\frac12\hbar\omega\frac{d^2\psi}{du^2}
+\frac12\hbar\omega u^2\psi(u) =E\psi(u) $$ $$ -\frac{d^2\psi}{du^2} + u^2\psi(u) =
\frac{2E}{\hbar\omega}\psi(u) $$

The left part of the equation is dimensionless. This forces us to interpret the quantity $2E/\hbar\omega$ as also dimensionless. For ease of calculations we consider it as some dimensionless energy $\mathcal E$.

$$ \boxed{\mathcal{E}:=\frac{2E}{\hbar\omega}} $$

Because we included the factor of 2 in the dimensionless energy, this will result in it missing from equation (2).

$$\boxed{\frac{d^2\psi}{du^2}=\left(u^2-\mathcal{E}\right)\psi(u)}\tag{3}$$

"Brute Force" Solution

There doesn't seem to be some obvious solution for (3). In reality a solution doesn't exist for all possible energies, since the squared term blows the wavefunction to infinity for large enough u, making it impossible to normalize.

We can find the form of the solutions by studying how the equation behaves when $u\to\pm\infty$.

$$\frac{d^2\psi}{du^2}=u^2\psi(u)$$

It seems like there isn't a pure polynomial solution, since the two parts of the equation will have a four

degree difference.

One can notice that the exponential $\left(e^{u^2}\right)'=2ue^{u^2}$ can increase the polynomial degree, and then try a solution in the form of ϕ below.

$$\phi(u)=u^ke^{\lambda u^2}$$ $$\phi'(u)=2\lambda u^{k+1}e^{\lambda u^2}+\dots = 2\lambda u\cdot\phi(u)+\dots$$ $$\phi''(u)=(2\lambda u)^2\cdot \phi(u)+\dots$$

For $\lambda=\pm1/2$ we have the form we need. So the solution could have the form:

$$\phi(u)\sim Au^{k}e^{-u^2/2}+Bu^ke^{u^2/2}$$

Now the problem of the solution blowing up to infinity is obvious. The second term of the sum cannot exist as a part of the wavefunction due to normalization constraints. We can suppose the form of the solution below:

$$\boxed{\psi(u)=h(u)\cdot e^{-u^2/2}} \tag{4}$$

$\phi(u)$ had a Au^k term where the power k was irrelevant, so we can interpret $h(u)$ as a power series.

$$h(u)=\sum_{n=0}^{\infty}a_nu^n$$

Replacing (4) in (3) will result in a differential equation with respect to $h(u)$, and solving it we can find the wavefuntion $\psi(u)$.

$$\frac{d^2\psi}{du^2}=(u^2-\mathcal{E})\psi(u)$$ $$\left[\frac{d^2h}{du^2}-2u\frac{dh}{du}+(u^2-1)h(u) \right]e^{-u^2/2} =(u^2-\mathcal{E})h(u)e^{-u^2/2} $$ $$\boxed{ \frac{d^2h}{du^2}-2u\frac{dh}{du}+(\mathcal{E}-1)h=0 } \tag{5} $$

Solving the Power Series DE

A simple replacement will result in a power series derivative, shifted starting point and a bunch of algebraic manipulation we can avoid. For a random $n\ge0$ some part of the power series will be:

$$h(u)=\ ...+a_nu^n+a_{n+1}u^{n+1}+a_{n+2}u^{n+2}+\dots$$

We can find the parts of the first and second derivative that end up with the same power and then sum them up accordingly.

$$\frac{d^2h}{du^2}=(n+2)(n+1)a_{n+2}u^n$$ $$-2u\frac{dh}{du}=-2na_nu^n$$ $$(\mathcal{E}-1)h=(\mathcal{E}-1)a_nu^n$$

Summing up the three terms above we can solve the DE and find the power series terms.

$$ \sum_{n=0}^\infty\Big[(n+2)(n+1)a_{n+2}-2na_n+(\mathcal E-1)a_n \Big]\cdot u^n=0 $$ $$(n+2)(n+1)a_{n+2}-(2n+1-\mathcal E)a_n=0$$ $$(n+2)(n+1)a_{n+2}=(2n+1-\mathcal E)a_n$$

$$\boxed{a_{n+2}=\frac{2n+1-\mathcal E}{(n+2)(n+1)}a_n} \tag{6}$$

With this recurrence relation we can find the whole function $h(u)$ if we only knew the first two terms, a_0 and a_1. The first one will give us all the even part of $h(u)$, and the second the odd

part. In order to find those terms, zeroing the function and its first derivative is enough.

$$h(0)=a_0+a_1\cdot0+a_2\cdot0^2+\ ...\ =a_0$$ $$h'(0)=a_1+2a_2\cdot0+3a_3\cdot0^2+\ ...\ =a_1$$

Making sure the solution converges

There still exists a problem. The series doesn't always converge. A simple ratio test can show that:

$$\left.\frac{a_{n+2}}{a_n}\right|_{n\to+\infty}=\frac{2n}{n^2}=\frac2n$$

The terms do get smaller, but not fast enough for convergence. It might not be obvious initially, but it can be shown that this is similar scaling to that of e^{u^2}, which for obvious reasons diverges.

$$\begin{align*} e^{u^2} &= \sum_{n=0}^\infty\frac{1}{n!}\left(u^2\right)^n \\ &= \sum_{n=0}^\infty\frac{1}{n!}u^{2n} \\ {\small(j=2n)}&=\sum_{j=0,2,4,\small\dots}^\infty\frac{1}{(j/2)!}u^j \\ &= \sum_{j=0,2,4,\small\dots}^\infty a_ju^j,\quad a_j=\frac{1}{(j/2)!} \end{align*}$$ We have to keep in mind since j is even, the factorial of $j/2$ is the factorial of a simple integer, so nothing fishy is happening here. Now, studying the limit at infinity we that we have the same scaling behaviour as above.

$$ \frac{a_{j+2}}{a_j} =\frac{(j/2)!}{\big((j+2)/2\big)!} =\frac{(j/2)!}{(j/2)!\cdot\big((j+2)/2\big)} =\frac{1}{\big((j+2)/2\big)} =\frac{2}{j+2} $$
$$\left.\frac{a_{j+2}}{a_j}\right|_{j\to+\infty}=\frac{2}{j}$$

We just proved that if the power series has infinite terms, the wavefunction at infinities would behave like below:

$$h(u)\propto e^{u^2},$$ $$\psi(u)\propto e^{u^2}\cdot e^{-u^2/2}=e^{u^2/2},\quad u\to\pm\infty \tag{7}$$

In such case the wavefunction can't be normalized, and thus cannot exist physically. The only way $h(u)$ has an acceptable form is if the power series terminates at some point, meaning $2n+1-\mathcal E=0$. Thus, **the energy is quantized**.

$$\boxed{\mathcal E_n=2n+1} \tag{8}$$

Replacing our definition for the dimensionless energy $(\mathcal E:=2E/\hbar\omega)$ we find the actuall energy levels in the real world.

$$\boxed{E_n=\left(n+\frac12\right)\hbar\omega} \tag{9}$$

An important note

There's no point in constructing a general solution $h(u)$ by mixing an even and an odd solution. The concept of eigenstate superposition regards the general solution of the time dependent Schrödinger equation. The differential equation of $h(u)$ is part of the eigenvalue problem of the time independent equation. In this case, the superposition of two eigenfunctions is not a solution to the eigenvalue problem

Mathematically this is expressed by the nature of the power series itself. If we have a mixed $h(u)$ with both odd and even parts, we can only have a single energy $\mathcal E$. This energy terminates only a single part of the series, either the odd or the even. This again results in the problem of (7), and $\psi(x)$ cannot be normalized. Thus we cannot mix an odd and an even $h(u)$ to find a more general solution.

Hermite polynomials

The different $h(u)$ functions that obey the restrictions above have been studied by mathematicians independently. They are called **Hermite Polynomials** and are denoted by $H_n(u)$. Per convention, and for ease of operations, they are usually written from largest to smallest power.

$$H_n(x)=(-1)^ne^{x^2}\frac{d^n}{dx^n}e^{-x^2}=2^nx^n+\ ...$$

These polynomials come from the solution of the Hermite differential equation. It so happens that our differential equation (5) above, when replacing the quantized energy (8) becomes the Hermite DE.

$$\frac{d^2H_n(u)}{du^2}-2u\frac{dH_n(u)}{du}+2nH_n(u)=0 \tag{10}$$

The first Hermite polynomials are:

$$H_0(u)=1$$ $$H_1(u)=2u$$ $$H_2(u)=4u^2-2$$ $$H_3(u)=8u^3-12u$$

The final result for the eigenfunctions is:

$$\psi_n(u)=N_nH_n(u)e^{-u^2/2},\quad u=\frac{x}{a}, a=\sqrt{\frac{\hbar}{m\omega}}$$

With proper normalization the wavefunctions are:

$$\boxed{ \psi_n(x)= \frac{1}{\sqrt{2^nn!}} \Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4} e^{\large-\frac{m\omega x^2}{2\hbar}} \ H_n\!\!\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \quad n=0,1,2,\dots\ }$$

$$\boxed{E_n=\hbar\omega\left(n+\frac12\right)}$$

Algebraic Solution

Starting from the Hamiltonian, we can write it as the sum of squares.

$$\hat H=\frac{\hat p^2}{2m}+\frac12m\omega^2\hat x^2=\frac12m\omega^2\left(\hat x^2+\frac{\hat p^2}{m^2\omega^2}\right)$$

We want to refactor it in a way that it stays hermitian. For any operator V the quantity $V^\dagger V$ is always hermitian, and an additive term μ doesn't affect the hermiticity, if $\mu\in\mathbb R$.

$$H=V^\dagger V+\mu$$

The form above makes solving any problem easier. Regarding the quantum harmonic oscillator, the two operators have a unique interpretation.

Trying to guess the operators

For the refactoring we can start by turning a sum of squares to a product of complex numbers.

$$a^2+b^2=(a-ib)\cdot(a+ib)$$

We then can guess some form of the refactored operators.

$$ \hat x^2+\frac{\hat p^2}{m^2\omega^2}\overset{?}{=} \left(\hat x-\frac{i\hat p}{m\omega}\right)\cdot \left(\hat x+\frac{i\hat p}{m\omega}\right) $$

The actual factorization won't be that, because we didn't take into consideration the fact that we have operators which don't commute. Starting with that guess though we can calculate the final from, also using the fact that $[\hat x,\hat p]=i\hbar$.

$$\begin{align*} \left(\hat x-\frac{i\hat p}{m\omega}\right) \cdot \left(\hat x+\frac{i\hat p}{m\omega}\right) &= \hat x^2+\frac{\hat p^2}{m^2\omega^2}+\frac{i}{m\omega}\left(\hat x\hat p-\hat p\hat x\right) \\ &= \hat x^2 + \frac{\hat p^2}{m^2\omega^2} + \frac{i}{m\omega}i\hbar \\ &= \hat x^2 + \frac{\hat p^2}{m^2\omega^2} - \frac{\hbar}{m\omega} \\ \\ &\Leftrightarrow \\ \\ \hat x^2 + \frac{\hat p^2}{m^2\omega^2} &= \underbrace{\left(\hat x-\frac{i\hat p}{m\omega}\right)}_{\Large V^\dagger}\cdot \underbrace{\left(\hat x+\frac{i\hat p}{m\omega}\right)}_{\Large V} +\frac{\hbar}{m\omega}\cdot\mathbb{I} \end{align*}$$ The real added term μ is $\hbar/m\omega$. Thus the Hamiltonian can be written as:

$$\hat H=\frac12m\omega^2\left(V^\dagger V+\frac{\hbar}{m\omega}\right)$$ $$\hat H=\frac12m\omega^2V^\dagger V+\frac12\hbar\omega \tag{11}$$

Construction & Annihilation operators

Ideally, we'd like to have these operators, $V^\dagger$ and V, in some type of normalized form. We can achieve that by studying their commutator.

$$\begin{align*} \left[V,V^\dagger\right] &= \left[\hat x+\frac{i\hat p}{m\omega},\hat x-\frac{i\hat p}{m\omega}\right] \\ &= -\frac{i}{m\omega}\left[\hat x,\hat p\right] + \frac{i}{m\omega}\left[\hat p,\hat x\right] \\ &= -\frac{i}{m\omega}\big(i\hbar-(-i\hbar)\big)\\ &= \frac{2\hbar}{m\omega} \\ \\ &\Leftrightarrow \left[\sqrt{\frac{m\omega}{2\hbar}}V,\sqrt{\frac{m\omega}{2\hbar}}V^\dagger\right]=1 \\ &\Leftrightarrow \left[\hat a, \hat a^\dagger\right] = 1 \end{align*}$$ $$$$

These are what we call the **creation** and **annihilation** operators $\hat a^\dagger, \hat a$. They are called this way because when they act on the Hamiltonian, they create or annihilate quanta of energy, one at a time, and thus raise or lower the energy state of the oscillator.

$$\boxed{\hat a^\dagger=\sqrt{\frac{m\omega}{2\hbar}}\left(\hat x-\frac{i}{m\omega}\hat p\right)}$$ $$\boxed{\hat a=\sqrt{\frac{m\omega}{2\hbar}}\left(\hat x+\frac{i}{m\omega}\hat

p\right)}$$ $$\left[\hat a,\hat a^\dagger\right]=1$$ $$\left[\hat a,\left(\hat a^\dagger\right)^n\right] = n\left(\hat a^\dagger\right)^{n-1}$$

Obviously those operators are not hermitian. But their combination is, just like $V^\dagger$ and V, since $\left(\hat a^\dagger\hat a\right)=\hat a^\dagger\left(\hat a^\dagger\right)^\dagger = \hat a^\dagger\hat a$. This factorization was first used by Paul Dirac and isn't limited to just the quantum harmonic oscillator. But their names are specific to the QHO, due to the quanta creation/annihilation. When used more generally they are called **ladder operators** as a pair, or **raising** and **lowering** operators when referring to them individually.

It is also useful to solve the system above for the position and momentum operators.

$$\boxed{\hat x=\sqrt{\frac{\hbar}{2m\omega}}\left(\hat a^\dagger+\hat a\right)}$$ $$\boxed{\hat p=i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat a^\dagger-\hat a\right)}$$

Rewriting the Hamiltonian

We can now write the Hamiltonian like this:

$$\begin{align*} \hat H &= \frac12m\omega^2V^\dagger V+\frac12\hbar\omega \\ &= \frac12m\omega^2\frac{2\hbar}{m\omega}\hat a^\dagger\hat a+\frac12\hbar\omega \\ &= \hbar\omega\hat a^\dagger\hat a+\frac12\hbar\omega \end{align*}$$ $$\boxed{\hat H=\hbar\omega\left(\hat a^\dagger\hat a+\frac12\right)}$$ $$$$

Here we can see for the first time that a **fundamental energy state** E_0 exists.

$$\begin{align*} \left<\hat H\right> &= \left<\psi\left|\hat H\right|\psi\right> \\ &= \left<\psi\left| \hbar\omega\left(\hat a^\dagger\hat a+\frac12 \right) \right|\psi\right> \\ &= \hbar\omega\left(\left<\psi\left|\hat a^\dagger\hat a\right|\psi\right> +\frac12\left<\psi|\psi\right> \right) \\ &= \hbar\omega\left(\left<\hat a\psi\big|\hat a\psi\right>+\frac12 \right) \ge \frac{\hbar\omega}{2} = E_0 \end{align*}$$ Requiring that the particle can take this fundamental energy gives us the form of the wavefunction. In order for $\left<\phi|\phi\right>=0$ it must be $\phi=0$ and thus $\hat a\psi_0(x)=0$.

$$\begin{align*} \hat a\psi_0(x) &= 0 \\ \sqrt{\frac{m\omega}{2\hbar}}\left(\hat x+\frac{i\hat p}{m\omega}\right)\psi_0(x) &= 0 \\ x\psi_0(x)+\frac{i}{m\omega}\cdot(-i\hbar)\frac{d\psi_0}{dx} &= 0 \\ x\psi_0(x)+\frac{\hbar}{m\omega}\frac{d\psi_0}{dx} &= 0 \\ \frac{d\psi_0}{dx} &= -\frac{m\omega}{\hbar}x\psi_0(x) \\ \\ \psi_0(x) &= Ce^{-\large\frac{m\omega}{2\hbar}\normalsize x^2} \end{align*}$$ After proper normalization, the fundamental wavefunction is: $$\boxed{ \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\large\frac{m\omega}{2\hbar}\normalsize x^2} }$$ ==== The Number Operator ==== The operator $\hat a^\dagger\hat a$ has a unique name. It's called the **number operator** and is denoted by $\hat N$. The Hamiltonian is also written $\hat H=\hbar\omega\left(\hat N+1/2\right)$. It's evident that they have the same eigenstates. Its function is to *label the energy level of a wavefunction*, meaning $\hat N\left|n\right>=n$. It can easily be shown that $\hat N\left|0\right>=\hat a^\dagger\left(\hat a\left|0\right>\right)=\hat a^\dagger\cdot0=0$, and thus:

$$\require{cancel} \hat H\left|0\right> = \hbar\omega\left(\cancelto{0}{\hat N\left|0\right>} + \frac12\left|0\right> \right) = \frac{\hbar\omega}{2}\left|0\right> $$

$$E_0=\frac{\hbar\omega}{2}$$

It's useful to study the behaviour of the number operator. This can be done by calculating its commutators.

$$ \big[\hat N,\hat a\big] =\big[\hat a^\dagger\hat a,\hat a\big] =\hat a^\dagger\big[\hat a,\hat a\big]+\big[\hat a^\dagger,\hat a\big]\hat a =0-\big[\hat a,\hat a^\dagger\big]\hat a =-\hat a $$

$$ \big[\hat N,\hat a^\dagger\big] =\big[\hat a^\dagger\hat a, \hat a^\dagger\big] =\hat a^\dagger\big[\hat a,\hat a^\dagger\big]+\big[\hat a^\dagger,\hat a^\dagger\big]\hat a =\hat a^\dagger\cdot 1+0 =\hat a^\dagger $$

$$\begin{align*} \big[\hat N,\hat a^k\big] &=\hat a^\dagger\big[\hat a,\hat a^k\big]+\big[\hat a^\dagger,\hat a^k\big]\hat a =0+\Big(\hat a^\dagger\hat a^k-\hat a^k\hat a^\dagger\Big)\hat a\\ &=\Big(\hat a^\dagger\hat a\hat a^{k-1}-\hat a^k\hat a^\dagger\Big)\hat a =\Big((\hat a\hat a^\dagger-1)\hat a^{k-1}-\hat a^k\hat a^\dagger\Big)\hat a\\ &=\Big(\hat a\hat a^\dagger\hat a^{k-1}-\hat a^k\hat a^\dagger-\hat a^{k-1}\Big)\hat a =\Big(\hat a(\hat a\hat a^\dagger-1)\hat a^{k-2}-\hat a^k\hat a^\dagger-\hat a^{k-1}\Big)\hat a\\ &=\Big(\hat a^2\hat a^\dagger\hat a^{k-2}-\hat a^k\hat a^\dagger-2\hat a^{k-1}\Big)\hat a =\big(\hat a^k\hat a^\dagger-\hat a^k\hat a^\dagger-k\hat a^{k-1}\Big)\hat a\\ &=-k\hat a^k \end{align*}$$ $$\begin{align*} \big[\hat N,(\hat a^\dagger)^k\big] &=\hat a^\dagger\big[\hat a,(\hat a^\dagger)^k\big]+\big[\hat a^\dagger,(\hat a^\dagger)^k\big]\hat a =\hat a^\dagger\Big(\hat a(\hat a^\dagger)^k-(\hat a^\dagger)^k\hat a\Big)+0\\ &=\hat a^\dagger\Big((\hat a^\dagger)^k\hat a-(\hat a^\dagger)^k\hat a+k(\hat a^\dagger)^{k-1}\Big) =\hat a^\dagger k(\hat a^\dagger)^{k-1}\\ &=k(\hat a^\dagger)^k \end{align*}$$

Excited states

How the construction and annihilation operators act on energy eigenstates

position and momentum operators

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