Class notes - MT tutorial 6

In our last tutorial this term we shall spend a great detail of time examining the quantum harmonic oscillator. To is hard to over-estimate quite how important the harmonic oscillator is. The concepts and methods learnt from it are essential, for example, in understanding quantum field theory.

1 A classical harmonic oscillator

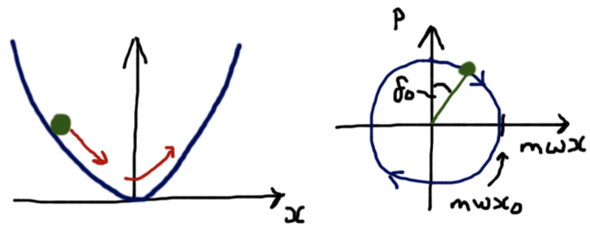
Let us begin by recalling some basic properties of a classical harmonic oscillator which you are all very familiar with. After solving the equation of motion

$$m\frac{\partial^2}{\partial t^2}x(t) = -kx(t),$$

we find that $x(t) = x_0 \sin(\omega t + \delta_0)$, where $\omega = \sqrt{k/m}$ while x_0 and δ_0 are the boundary conditions for the maximum displacement and initial momentum. Correspondingly the momentum can be solved as

$$p(t) = m\frac{\partial}{\partial t}x(t) = mx_0\omega\cos(\omega t + \delta_0).$$

As expected we find that the total energy $E = \frac{1}{2m}[p(t)^2 + m^2\omega^2 x(t)^2] = \frac{1}{2}m\omega^2 x_0^2$ is time-independent. An extremely compact way to visualise the dynamics of a harmonic oscillator is to plot the phase-space trajectory.



At any given time the phase space point for the system is given by the co-ordinates $\mathbf{p}(t) = (m\omega x(t), p(t))$, and with the solution given can be seen that $\mathbf{p}(t)$ traces out a circle of radius $m\omega x_0$ (the turning points). Thus the dynamics of a harmonic oscillator is completely characterised by a point which moves clockwise around the circle. We shall return to this phase space picture later and see how similar the quantum mechanical version is.

2 Observations for the quantum case

The Hamiltonian for a particle in a harmonic oscillator (parabolic) potential has the obvious form

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2.$$

Notice that in contrast to the particle in a infinite box the motion of the particle is not restricted to a finite-region. We therefore expect that stationary states will have wave functions obeying $\psi(|x| \to \infty) \to 0$. An important property of $\hat{H}$ for a harmonic oscillator is that for any state $|\psi\rangle$ it obeys $\langle\psi|\hat{H}|\psi\rangle \geq 0$, which indicates that the ground state energy must be non-negative[1]. This can be shown very easily by noting that

$$\frac{1}{2m}\underbrace{\langle\psi|\hat{p}^2|\psi\rangle}_{\geq 0} + \tfrac{1}{2}m\omega^2\underbrace{\langle\psi|\hat{x}^2|\psi\rangle}_{\geq 0} \geq 0,$$

since for any hermitian operator $\hat{B}$ we have $\langle\psi|\hat{B}^2|\psi\rangle = (\langle\psi|B^\dagger)(B|\psi\rangle) = \langle\phi|\phi\rangle$ where $|\phi\rangle = B|\psi\rangle$, so the result follows from the basic property of the scalar-product that $\langle\phi|\phi\rangle \geq 0$ for any state $|\phi\rangle$. We could have also guessed this result by the fact that classically the harmonic potential never drops below zero.

To solve for the eigenstates of the harmonic oscillator we must solve the eigenvalue problem for

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) + \tfrac{1}{2}kx^2\phi(x) = E\phi(x). \tag{1}$$

This equation can be rescaled by defining a dimensionless quantity $y = x/a_{\rm ho}$, where $a_{\rm ho} = \sqrt{\hbar/m\omega}$ is the harmonic oscillator length scale. This gives

$$\frac{\hbar\omega}{2}\left(-\frac{\partial^2}{\partial y^2}\phi(y) + y^2\phi(y)\right) = E\phi(y). \tag{2}$$

It can easily be verified that a gaussian $\phi(y) = A\exp(-\frac{1}{2}y^2)$, where A is a normalisation constant, is a solution of this equation if $E = \frac{1}{2}\hbar\omega$. While this is an eigenstate what we now need to determine is whether it is the ground state and also what the other eigenstates are.

3 Conventional ODE method

In an entirely analogous way to how we approached the particle in a box we can sit down and try to solve by brute force[2] the ODE in Eq. (2). You can find this explained in great detail in many quantum mechanics textbooks so here I will simply review the results. Firstly given our trial gaussian solution above we attempt an ansatz $\phi(y) = h(y)\exp(-\frac{1}{2}y^2)$, where $h(y)$ is some polynomial in y. Inserting this into Eq. (2) gives

$$\frac{\hbar\omega}{2}e^{-\frac{y^2}{2}}\left(-\frac{\partial^2}{\partial y^2}h(y) + 2y\frac{\partial}{\partial y}h(y) + h(y)\right) = Eh(y)e^{-\frac{y^2}{2}}.$$

from which we obtain Hermite's equation

$$\frac{\partial^2}{\partial y^2}h(y) - 2y\frac{\partial}{\partial y}h(y) + \left(\frac{2E}{\hbar\omega} - 1\right)h(y) = 0. \tag{3}$$

This equation can be solved to obtain an infinite sequence of orthogonal polynomials $h_n(y)$, i.e. $\int_{-\infty}^{\infty} dy h_n^*(y)h_m(y) = \delta_{nm}$. This is expected since the problem is of Sturm-

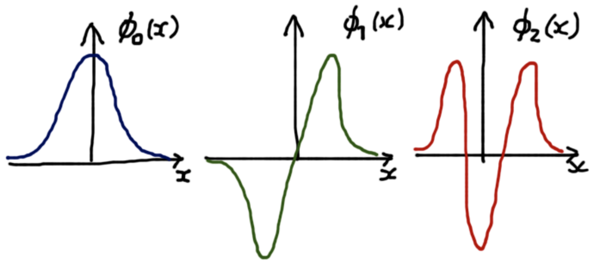
[1] In general, there is nothing physically wrong with having a negative energy, since it depends only on where you put the zero energy reference. In the oscillators case we choose the zero to be the bottom of the potential. As we shall see next term convenience dictates that for hydrogen the zero energy is when it is ionised so the ground state has an energy of $\varepsilon = -13.6$ eV.

[2] Also known as the *boring* method.

Liouville form and should have orthogonal eigenfunctions. The first few hermite polynomials are

$$\begin{aligned} h_0(y) &= 1, \\ h_1(y) &= 2y, \\ h_2(y) &= 4y^2 - 2, \\ h_3(y) &= 8y^3 - 12y, \\ &\vdots \end{aligned}$$

The eigenstates of the harmonic oscillator are then $\phi_n(y) = h_n(y)\exp(-\frac{1}{2}y^2)$, labelled by an integer $n = 0, 1, 2, \cdots$, with energies $E_n = \hbar\omega(n + \frac{1}{2})$. The first three eigenstates are sketched very roughly here



Notice that the nth eigenstate is a gaussian modulated by a polynomial of degree n and so n labels the number of nodes of the wave-function and also the parity (mirror symmetry) which goes as $(-1)^n$. The gaussian wave-function is the ground state, as one might expect, since it has the least number of nodes (recall that kinetic energy increases the more a wave-function oscillates) out of all the eigenstates.

4 Operator method

While we do in principle learn all the essential information from the conventional approach there is a far more elegant approach to the harmonic oscillator which exposes its full structure and more generally provides a highly abstract way to view its solution. To begin we note that the Hamiltonian for the harmonic oscillator is a differential operator

$$\frac{\hat{H}}{\hbar\omega} = \frac{1}{2}\left(-\frac{\partial^2}{\partial y^2} + y^2\right).$$

We can now factorise this operator by defining two new operators whose product reconstructs $\hat{H}$ as

$$\hat{A}^\dagger = \frac{1}{\sqrt{2}}\left(-\frac{\partial}{\partial y} + y\right), \quad \text{and} \quad \hat{A} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial y} + y\right).$$

It can easily be verified that $\hat{H} = \hbar\omega(\hat{A}^\dagger\hat{A} + \frac{1}{2})$, and also that $\hat{A}^\dagger$ really is the hermitian conjugate differential operator of $\hat{A}$ as the notation suggests. However, since $\hat{A}^\dagger \neq \hat{A}$ we see they are not themselves hermitian operators. Note that for any operator $\hat{B}$ (not necessarily hermitian) the product $\hat{B}^\dagger\hat{B}$ is hermitian and moreover is a positive hermitian operator, by which we mean that it has a non-negative eigen-spectrum. The proof of this is identical to that used earlier, namely $\langle\psi|\hat{B}^\dagger\hat{B}|\psi\rangle = (\langle\psi|B^\dagger)(B|\psi\rangle) \geq 0$. This means that our factorisation has refined our lower-limit on the energy of a harmonic oscillator as $\langle\hat{H}\rangle \geq \frac{1}{2}\hbar\omega$. This is not something which could be guessed classically and indicates that the ground state must have a non-zero energy. In fact we know already that the ground state energy precisely saturates this lower-bound and the finite residual energy is sometimes called the zero-point energy (we'll say more about this shortly). The operators $\hat{A}^\dagger$ and $\hat{A}$ can readily recast in terms of more intuitive position and momentum operators as

$$\hat{A}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2m\omega\hbar}}\hat{p}, \quad \text{and} \quad \hat{A} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2m\omega\hbar}}\hat{p},$$

showing that they are linear combinations of $\hat{x}$ and $\hat{p}$.

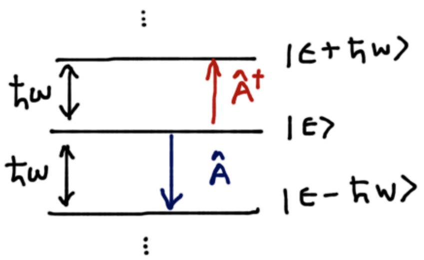
The utility of introducing $\hat{A}^\dagger$ and $\hat{A}$ is that the solution to the harmonic oscillators eigenstates and eigenvalues follows from some simple algebra. Firstly we note that $[\hat{A},\hat{A}^\dagger] = 1$, from which it follows that

$$\begin{aligned} [\hat{H},\hat{A}] &= -\hbar\omega\hat{A}, \\ [\hat{H},\hat{A}^\dagger] &= \hbar\omega\hat{A}^\dagger. \end{aligned}$$

Now suppose we have some state $|\varepsilon\rangle$ which is an eigenstate of $\hat{H}$ satisfying $\hat{H}|\varepsilon\rangle = \varepsilon|\varepsilon\rangle$. We can then form some new (not normalised) state $\hat{A}^\dagger|\varepsilon\rangle$ and we can find via the commutation relations that

$$\hat{H}\hat{A}^\dagger|\varepsilon\rangle = (\hat{A}^\dagger\hat{H} + \hbar\omega\hat{A}^\dagger)|\varepsilon\rangle = (\varepsilon + \hbar\omega)\hat{A}^\dagger|\varepsilon\rangle,$$

and so $\hat{A}^\dagger|\varepsilon\rangle$ is also an eigenstate of $\hat{H}$ but with an eigenvalue $\varepsilon + \hbar\omega$. The application of the operator $\hat{A}^\dagger$ has raised the energy of an (arbitrary) eigenstate $|\varepsilon\rangle$ by one unit of $\hbar\omega$ and for this reason is called the *raising operator*. A similar calculation reveals that $\hat{H}\hat{A}|\varepsilon\rangle = (\varepsilon - \hbar\omega)\hat{A}|\varepsilon\rangle$. Thus $\hat{A}|\varepsilon\rangle$ is also an eigenstate of $\hat{H}$ but with an eigenvalue $\varepsilon - \hbar\omega$ and correspondingly $\hat{A}$ is called a *lowering* operator. This can be summarised by the picture



Given that $\hat{A}$ lowers the energy by one unit of $\hbar\omega$ we know that it cannot do this indefinitely since we have lower bounded the spectrum of $\hat{H}$ to be $\frac{1}{2}\hbar\omega$. This means that the ladder of eigenstates we descend by using $\hat{A}$ must terminate with some state $|\phi_0\rangle$ as $\hat{A}|\phi_0\rangle = 0$. We can express this equation as a differential equation acting on a wave-function as

$$\langle y|\hat{A}|\phi_0\rangle = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial y} + y\right)\phi_0(y) = 0.$$

This can be readily solved to give the gaussian $\phi_0(y) = A\exp(-\frac{1}{2}y^2)$ again as the ground state with an energy $\frac{1}{2}\hbar\omega$. Having determined one state in the ladder (the bottom one) we can construct all the other (not normalised) eigenfunctions by the repeated application of $\hat{A}^\dagger$ as $\phi_n(y) = (\hat{A}^\dagger)^n \phi_0(y)$, and immediately know that all eigenstates are equally spaced and that they differ in energy by n units of $\hbar\omega$ from $\phi_0(y)$. This gives $E_n = \hbar\omega(n + \frac{1}{2})$, as stated earlier. Notice that when expressed as differential operators acting on the ground state wave-function we obtain

$$\begin{aligned}
\phi_1(y) &= \left(-\frac{\partial}{\partial y} + y\right)\phi_0(y) = 2ye^{-\frac{y^2}{2}}, \\
\phi_2(y) &= \left(-\frac{\partial}{\partial y} + y\right)^2 \phi_0(y) = 2(2y^2 - 1)e^{-\frac{y^2}{2}}, \\
&\vdots
\end{aligned}$$

and so the hermite polynomials from the conventional approach are automatically generated by this operator procedure.

5 Properties of the ground state

As was mentioned before the lowest energy of the quantum harmonic oscillator is nonzero. This is a general quantum phenomena which we have encountered already in the infinite box potential. Clearly this is related to Heisenberg's uncertainty principle and this can be revealed in a very transparent way for the harmonic oscillator. Now classically we expect the ground state to be a particle with position $x = 0$ and momentum $p = 0$, but quantum mechanically this intuition can only be translated into $\langle \hat{x} \rangle = 0$ and $\langle \hat{p} \rangle = 0$. This is certainly confirmed by the gaussian ground state found in our earlier calculations but here we are simply conjecturing it on more general grounds and want to see how much we can figure out without assuming the answer already. Due to these zero averages we have that $\Delta(\hat{x})^2 = \langle \hat{x}^2 \rangle$ and $\Delta(\hat{p})^2 = \langle \hat{p}^2 \rangle$ thus the expectation value of the energy becomes directly dependent[3] on the position and momentum fluctuations as

$$\langle \hat{H} \rangle = \frac{1}{2m}\left[\Delta(\hat{p})^2 + \Delta(m\omega\hat{x})^2\right].$$

We can then see that $\langle \hat{H} \rangle = 0$ is not permitted quantum mechanically since it necessitates zero fluctuations. We can work out the minimum energy that is allowed quantum mechanically by assuming that the ground state satisfies $\Delta(m\omega\hat{x})\Delta(\hat{p}) = \frac{1}{2}m\hbar\omega$. To do this we assume that

$$\Delta(\hat{p}) = Q^{\frac{q}{2}}, \quad \text{and} \quad \Delta(m\omega\hat{x}) = Q^{1-\frac{q}{2}}, \quad \text{with} \quad Q = \frac{m\hbar\omega}{2},$$

and therefore allow for the possibility, through the exponent q, that our ground state may have an arbitrary fluctuations in position and momentum such that their product saturates the uncertainty principle. In the end we get a q dependent energy expectation value

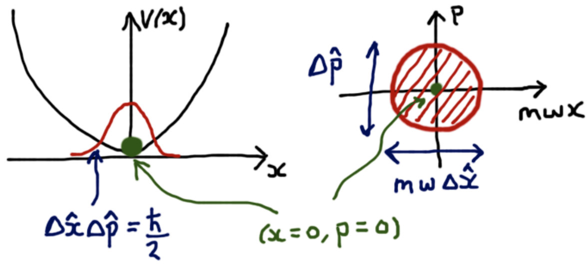
$$\langle \hat{H}(q) \rangle = \frac{1}{2m}\left(Q^q + Q^{2-q}\right).$$

[3] This relationship between energy and fluctuations is because the harmonic oscillator is quadratic in $\hat{x}$ and $\hat{p}$. Other potentials will not have such a simple and direct relation.

We now want to find the distribution of fluctuations q which minimises this energy and so compute

$$\frac{d}{dq}\langle\hat{H}(q)\rangle = \ln(Q)Q^q - \ln(Q)Q^{2-q},$$
$$\frac{d^2}{dq^2}\langle\hat{H}(q)\rangle = \ln(Q)^2Q^q + \ln(Q)^2Q^{2-q}.$$

Since $\ln(Q) \neq 0$ solving $\frac{d}{dq}\langle\hat{H}(q)\rangle = 0$ gives $Q^q = Q^{2-q}$ and hence the exponent $q = 1$. Since the second derivative is positive for this value of q this solution is a genuine minima for the energy $\langle\hat{H}(q)\rangle$ and thus shows that the fluctuations in $\Delta(m\omega\hat{x})$ and $\Delta(\hat{p})$ are equal. As we have seen last week the gaussian wave-function is precisely the state which both minimises and equalises the position and momentum uncertainties. The ground state of the harmonic oscillator is therefore uniquely determined by the uncertainty principle and can represented in phase space as a circular region about the origin (the point at the origin being the classical ground state) of radius $\sqrt{\frac{1}{2}m\hbar\omega}$.

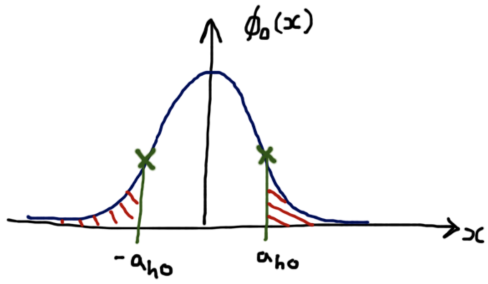


This zero-point motion / zero-point energy has measurable consequences. In particular it prevents Helium from freezing. Helium instead remains a liquid at $T = 0$ for reasonable situations, and instead requires extreme pressure to solidify. This occurs because the zero-point motion of the Helium atoms is enough to overcome the very weak van-der-Waal attraction between them.

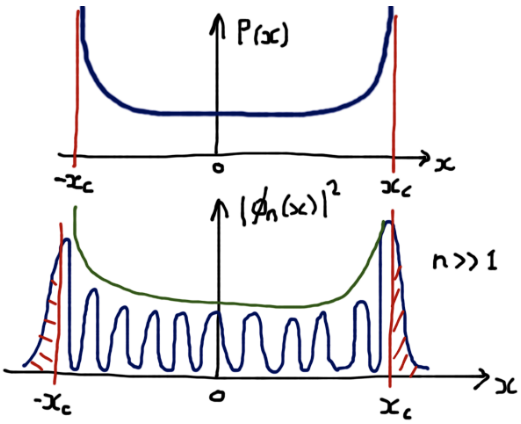
In addition to finding a non-zero energy the quantum ground state deviates from expected classical motion even if we account for the non-zero energy. For a classical particle with a total energy $E = \frac{1}{2}\hbar\omega$ it will always be confined to a region $-a_{\rm ho} \leq x \leq a_{\rm ho}$, where $a_{\rm ho}$ is the harmonic oscillator length defined earlier. For such a particle oscillating backwards and forwards we can construct a probability distribution for how likely we are to find a particle at a given position x (were we to take a look at some random time) as

$$p(x) \propto \frac{1}{\sqrt{a_{\rm ho}^2 - x^2}}.$$

From the time-independent Schrodinger equation Eq. (1) when $E = \frac{1}{2}\hbar\omega$ we find that the points of inflection $\frac{d^2}{dx^2}\phi_0(x) = 0$ of the ground state also occur at $x = a_{\rm ho}$. It is then clear that the gaussian ground state wave-function for the quantum case significantly overshoots the classical turning points.

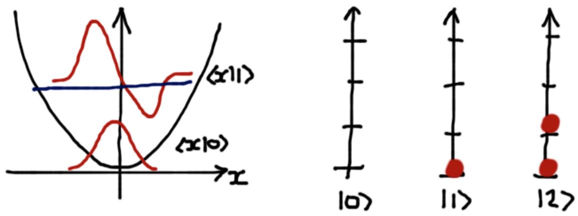


This overshooting is also found for the nth eigenstate. However, in agreement with the correspondence principle it is found that $|\phi_n(x)|^2$ becomes increasingly similar to $p(x)$, with a vanishing probability beyond the classical turning point $x_c = a_{\rm ho}\sqrt{2n+1}$, as $n \rightarrow \infty$.



6 Abstract interpretation

The picture we have had so far has been firmly fixed to a particle trapped in a one-dimensional parabolic potential. However, the harmonic oscillator is far more general then this and to reveal this the operator framework created earlier is often written in a slightly more abstract way. Indeed we can instead view the harmonic oscillator as a many-particle problem and use it to form the basis of what is often called *second quantisation*. In this picture the ground state of the harmonic oscillator contains no quanta (particles), with the nth eigenstate contains n quanta each with energy $\hbar\omega$. This abstract interpretation is sensible only because the harmonic oscillator spectrum increases linearly with n exactly as one would expect if we added quanta. To formalise this we label the eigenstate as a ket $|n\rangle$, where $n = 0, 1, 2, \ldots$ is the number of quanta (or units of energy in $\hbar\omega$ above the zero-point energy), so the ground state (or vacuum state) is now denoted as $|0\rangle$. Keep in mind though that $|0\rangle$ is a genuine quantum state (a gaussian wave-function for a particle) and **not** the null vector.



We then create all the other eigenstates by apply the *creation* operator $A^\dagger$ to the empty vacuum state to create quanta as

$$|n\rangle = \frac{(\hat{A}^\dagger)^n}{\sqrt{n!}}|0\rangle.$$

The normalisation for the state $|n\rangle$ used above is computed in QMMT Q6.4. We also have the *annihilation* operator $\hat{A}$ which removes quanta until the system has no more. Together the creation and annihilation operators obey $[\hat{A},\hat{A}^\dagger] = 1$ which is called the canonical bosonic commutation relation. Bosons and fermions will be dealt with more later in the year and in the Statistical mechanics course, but we can see currently that our operator algebra permits many quanta so we don't expect this to describe fermions which obey the Pauli exclusion principle. The action of the creation and annihilation operators on the eigenstates is best summarised as

$$\begin{aligned}\hat{A}|n\rangle &= \sqrt{n}|n-1\rangle,\\ \hat{A}^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle,\end{aligned}$$

from which we see that $\hat{A}^\dagger\hat{A}|n\rangle = n|n\rangle$, so $\hat{A}^\dagger\hat{A}$ simply counts the number of quanta in our eigenstate. For this reason $\hat{n} = \hat{A}^\dagger\hat{A}$ is often called the number operator and the Hamiltonian for a harmonic oscillator is simply

$$\hat{H} = \hbar\omega(\hat{n} + \tfrac{1}{2}).$$

Eigenstates of $|n\rangle$ are also called number states because they possess a precise well defined number of quanta. We can form a concrete representation of the operators $\hat{n}$, $\hat{A}$, and $\hat{A}^\dagger$ in the number basis using $\langle n'|\hat{n}|n\rangle = n\delta_{n',n}$ as

$$\hat{n} = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & \cdots \\ 0 & 0 & 0 & 3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

along with $\langle n'|\hat{A}|n\rangle = \sqrt{n}\delta_{n',n-1}$ as

$$\hat{A} = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ 1 & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

and $\langle n'|\hat{A}^\dagger|n\rangle = \sqrt{n+1}\,\delta_{n',n+1}$ as

$$\hat{A}^\dagger = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & \cdots \\ 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

This abstract formalism is a basic tool used in quantum field theory to perform, for example, the canonical quantisation of the electromagnetic field or of lattice vibrations. Specifically, we can attach a harmonic oscillator with its own operators $\hat{a}^\dagger_{\mathbf{k},\omega}$ and $\hat{a}_{\mathbf{k},\omega}$ to each mode $(\mathbf{k},\omega)$ of the electromagnetic field (or of acoustic waves), with the corresponding quanta being photons in that specific mode (or phonons for sound). We won't pursue this here, but rest assured the harmonic oscillator will return in your future work in this context. Instead we will continue to discuss a particle in a harmonic trap but will find it convenient to sometimes phrase things using the abstract quanta terminology.

With the operator formalism we can now compute in a very straightforward way the fluctuations of number states $|n\rangle$. In the context of a particle in a harmonic potential we want to know $\Delta(\hat{x})$ and $\Delta(\hat{p})$ for the nth eigenstate? To do this calculation we note first that

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{A}+\hat{A}^\dagger) \quad \text{and} \quad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}(\hat{A}-\hat{A}^\dagger).$$

It is then immediately obvious that $\langle n|\hat{x}|n\rangle = 0$ and $\langle n|\hat{p}|n\rangle = 0$ since $\hat{A}|n\rangle \propto |n-1\rangle$ and $\hat{A}^\dagger|n\rangle \propto |n+1\rangle$ and $|n\rangle$ is orthogonal to both $|n-1\rangle$ and $|n+1\rangle$ (identically we see that $\hat{x}$ and $\hat{p}$ when written as matrices have no diagonal elements in the number basis, or in terms of wave-functions the integrals have odd integrands integrated over a symmetric interval). In fact more generally we know that $\langle n|\hat{A}^k|n\rangle = 0$ along with $\langle n|(\hat{A}^\dagger)^k|n\rangle = 0$, for any integer k, for the same reason. We now want to compute the diagonal matrix elements in the number basis of $\hat{x}^2$ and $\hat{p}^2$ which we can do by first reorganising the operators as

$$\hat{x}^2 = \frac{\hbar}{2m\omega}(\hat{A}+\hat{A}^\dagger)^2 = \frac{\hbar}{2m\omega}(\hat{A}^2+(\hat{A}^\dagger)^2+2\hat{A}^\dagger\hat{A}+1),$$

and

$$\hat{p}^2 = -\frac{m\hbar\omega}{2}(\hat{A}-\hat{A}^\dagger)^2 = -\frac{m\hbar\omega}{2}(\hat{A}^2+(\hat{A}^\dagger)^2-2\hat{A}^\dagger\hat{A}-1),$$

where we have used the canonical commutation relation. From our earlier reasoning we see immediately that

$$\langle n|\hat{x}^2|n\rangle = \frac{\hbar}{2m\omega}(2n+1), \quad \text{and} \quad \langle n|\hat{p}^2|n\rangle = \frac{m\hbar\omega}{2}(2n+1).$$

Since $\langle\hat{x}\rangle = \langle\hat{p}\rangle = 0$ we have that $\Delta(\hat{x})^2 = \langle\hat{x}^2\rangle$ and $\Delta(\hat{p})^2 = \langle\hat{p}^2\rangle$ giving

$$\Delta(\hat{x})\Delta(\hat{p}) = \hbar(n+\tfrac{1}{2}),$$

as the uncertainty relation for $|n\rangle$. It is hard to imagine this same calculation using integration of harmonic oscillator wave-functions could ever be this simple! Thus we see that the position and momentum uncertainty increase linearly with the number of quanta and is clearly minimised for the ground state where $n = 0$. In phase space we can therefore visual the state $|n\rangle$ as a circle of radius $\sqrt{m\hbar\omega(n+\frac{1}{2})}$. Since number states are stationary states of $\hat{H}$ they don't display any time-dependent motion for $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$ and so do not reproduce the dynamics we would normally associate to a particle in a harmonic potential classically, namely rolling back and forth. In the last section of these notes we shall construct quantum states of the harmonic oscillator whose properties do resemble classical motion as closely as is possible.

7 Coherent states

This section is **not** examinable, however the discussion below is physically intuitive and may well help you "guess" what answers to expect in some exam questions. Mathematically coherent states are defined as the right eigenvectors[4] of the annihilation (lowering) operator $\hat{A}$, specifically states obeying

$$\hat{A}\,|\alpha\rangle = \alpha\,|\alpha\rangle\,.$$

Here the eigenvalue α is in general a complex number since $\hat{A}$ is not hermitian. We want to know what values α is permitted to take and what the associated eigenstates states $|\alpha\rangle$ are. To do this we first expand an arbitrary $|\alpha\rangle$ in the number basis

$$|\alpha\rangle = \sum_{n=0}^{\infty} c_n\,|n\rangle = \overbrace{\left(\sum_{n=0}^{\infty} c_n \frac{(\hat{A}^\dagger)^n}{\sqrt{n!}}\right)}^{f(\hat{A}^\dagger)}|0\rangle\,,$$

from which we see that any state $|\alpha\rangle = f(\hat{A}^\dagger)\,|0\rangle$ where $f(a)$ is a regular power-series function of its argument a highlighted above. The eigenvalue equation defining a coherent state is then

$$\hat{A}f(\hat{A}^\dagger)\,|0\rangle = \alpha f(\hat{A}^\dagger)\,|0\rangle\,.$$

In Gasiorowicz Q6.4 the following identity was proven

$$\hat{A}f(\hat{A}^\dagger)\,|0\rangle = \frac{df(\hat{A}^\dagger)}{d\hat{A}^\dagger}\,|0\rangle\,,$$

which states that the action of $\hat{A}$ on any function of $\hat{A}^\dagger$ sandwiched between it and the vacuum $|0\rangle$ is to formally differentiate that function with respect to its argument (in this case an operator). This gives us a differential equation

$$\frac{df(a)}{da} = \alpha f(a),$$

which can be easily solved as $f(a) = Ce^{\alpha a}$, with C being a constant. Thus a coherent state has the form where $f(a)$ is a exponential of the creation operator as

$$|\alpha\rangle = Ce^{\alpha\hat{A}^\dagger}\,|0\rangle\,.$$

[4]For an hermitian operator $\hat{B}$ we don't bother distinguishing between left and right eigenvectors since if $|b\rangle$ is a right eigenstate it obeys $\hat{B}|b\rangle = b|b\rangle$ then it also obeys $\langle b|\hat{B} = b\langle b|$, since b is real, and is a left eigenvector automatically. Since $\hat{A}$ is not hermitian we cannot assume this.

Our calculation has revealed no restrictions on α, it can be any complex number, and so there are an infinite and continuous set of right eigenstates[5] $|\alpha\rangle$ of $\hat{A}$. The term "right" eigenstates has been stressed since $\hat{A}|\alpha\rangle = \alpha|\alpha\rangle$ does not imply $\langle\alpha|\hat{A} = \alpha\langle\alpha|$ as one would have for hermitian operators. Coherent states are not left eigenstates of $\hat{A}$, rather by hermitian conjugating the right eigenvalue equation for $\hat{A}$ we get $\langle\alpha|\hat{A}^\dagger = \alpha^*\langle\alpha|$, so they are left eigenstates of the creation operator $\hat{A}^\dagger$.

To complete our calculation of coherent states we need to determine the normalisation constant C. Computing $\langle\alpha|\alpha\rangle = 1$ gives

$$\begin{aligned} |C|^2\langle 0|e^{\alpha^*\hat{A}}e^{\alpha\hat{A}^\dagger}|0\rangle &= 1, \\ |C|^2\langle 0|\sum_{n=0}^{\infty}\frac{(\alpha^*)^n}{n!}\left(\frac{d}{d\hat{A}^\dagger}\right)^n e^{\alpha\hat{A}^\dagger}|0\rangle &= 1, \\ |C|^2\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!}\langle 0|e^{\alpha\hat{A}^\dagger}|0\rangle &= 1, \end{aligned}$$

but since $\langle 0|e^{\alpha\hat{A}^\dagger}|0\rangle = \langle 0|\mathbb{1} + \alpha\hat{A}^\dagger + \frac{1}{2}\alpha^2(\hat{A}^\dagger)^2 + \ldots|0\rangle = \langle 0|0\rangle = 1$ this reduces to

$$\begin{aligned} |C|^2\sum_{n=0}^{\infty}\frac{|\alpha|^{2n}}{n!} &= 1, \\ |C|^2 e^{|\alpha|^2} = 1, \end{aligned}$$

so $|C| = \exp(-\frac{1}{2}|\alpha|^2)$ and properly normalised coherent states are (up to a global phase)

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}}e^{\alpha\hat{A}^\dagger}|0\rangle.$$

Once normalised we can use the defining properties of coherent states to compute many quantities trivially. For example the average number of quanta follows easily from

$$\langle\alpha|\hat{n}|\alpha\rangle = \overbrace{\langle\alpha|\hat{A}^\dagger}^{\alpha^*\langle\alpha|}\overbrace{\hat{A}|\alpha\rangle}^{|\alpha\rangle\alpha} = |\alpha|^2\langle\alpha|\alpha\rangle = |\alpha|^2,$$

while the number fluctuations can be found from

$$\begin{aligned} \langle\alpha|\hat{n}^2|\alpha\rangle &= \langle\alpha|\hat{A}^\dagger\hat{A}\hat{A}^\dagger\hat{A}|\alpha\rangle, \\ &= \langle\alpha|\hat{A}^\dagger\hat{A}^\dagger\hat{A}\hat{A} + \hat{A}^\dagger\hat{A}|\alpha\rangle, \\ &= |\alpha|^4 + |\alpha|^2 = \langle\hat{n}\rangle^2 + \langle\hat{n}\rangle, \end{aligned}$$

so $\Delta(\hat{n}) = \sqrt{\langle\hat{n}\rangle}$. We can now work out more precisely what probability distribution over the number basis generates this kind of mean and fluctuation by first expanding the exponential

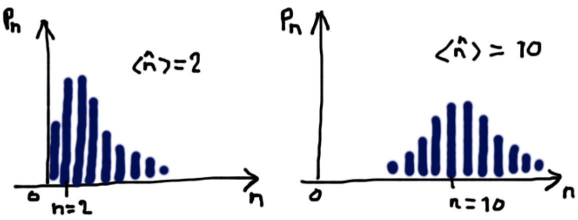
$$\begin{aligned} |\alpha\rangle &= e^{-\frac{|\alpha|^2}{2}}e^{\alpha\hat{A}^\dagger}0, \\ &= e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{(\alpha\hat{A}^\dagger)^n}{n!}|0\rangle, \\ &= e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle. \end{aligned}$$

[5] The set of coherent states $|\alpha\rangle$ coincide with number states $|n\rangle$ only when $\alpha = 0$ since $|\alpha = 0\rangle = |0\rangle$, but should α ever equal any other integer n the resulting coherent state does not correspond to a number state, so $|\alpha = n\rangle \neq |n\rangle$, as can be readily seen from its expansion in the number basis.

This shows that coherent states with $|\alpha| > 0$ are a weighted superpositions of all the number states $|n\rangle$. The probability distribution P_n for a coherent state to possess precisely n quanta is then simply

$$P_n = |\langle n|\alpha\rangle|^2 = \frac{|\alpha|^{2n}}{n!}e^{-|\alpha|^2}.$$

Given that $|\alpha|^2 = \langle\hat{n}\rangle$ we see that $P_n = \langle\hat{n}\rangle^{2n}e^{-\langle\hat{n}\rangle}/n!$ is a Poisson number distribution.



Thus $|\alpha|^2$ determines where the distribution is peaked and the fractional uncertainty of this peak is

$$\frac{\Delta(\hat{n})}{\langle\hat{n}\rangle} = \frac{1}{\sqrt{\langle\hat{n}\rangle}},$$

showing that relative to its average quanta number its fluctuations decrease as the average number of quanta increases.

So what has any of this got to do with classical motion? To make this connection let's compute the position and momentum of a coherent state along with their fluctuations so we can view them in phase space. We find that

$$\langle\alpha|\hat{x}|\alpha\rangle = \frac{a_{\rm ho}}{\sqrt{2}}(\alpha+\alpha^*) = a_{\rm ho}\sqrt{2}\,\mathrm{Re}(\alpha), \tag{4}$$

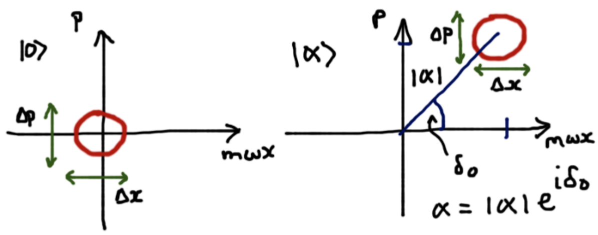
$$\langle\alpha|\hat{p}|\alpha\rangle = i\frac{\hbar}{a_{\rm ho}\sqrt{2}}(\alpha^*-\alpha) = \frac{\hbar}{a_{\rm ho}}\sqrt{2}\,\mathrm{Im}(\alpha), \tag{5}$$

so $|\alpha\rangle$ generally has a non-zero position and momentum given by its real and imaginary components, respecitvely, along with

$$\langle\alpha|\hat{x}^2|\alpha\rangle = \frac{a_{\rm ho}^2}{2}[\alpha^2+(\alpha^*)^2+2|\alpha|^2+1],$$

$$\langle\alpha|\hat{p}^2|\alpha\rangle = -\frac{\hbar^2}{2a_{\rm ho}^2}[\alpha^2+(\alpha^*)^2-2|\alpha|^2-1].$$

This then gives position and momentum fluctuations $\Delta(\hat{x})^2 = a_{\rm ho}^2/2$ and $\Delta(\hat{p})^2 = \hbar^2/2a_{\rm ho}^2$, which are both independent of α and satisfy $\Delta(\hat{x})\Delta(\hat{p}) = \frac{1}{2}\hbar$. Coherent state therefore have the same minimum and equal uncertainty in phase space as the vacuum (or ground state) only its centre is displaced from the origin.



This pleasing phase space picture in fact reveals how coherent states can be created physically. Suppose we have a particle trapped in a harmonic potential and we cooled it to the ground state $|0\rangle$. Then instantaneously we displace the harmonic potential along the x-axis by some distance. The wave-function of our particle is still in the gaussian ground state centred on the original minima but is now sitting "up the hill" in the new potential. If we express this original ground state wave-function in the basis of eigenstates of the new displaced harmonic potential it will be a coherent state. Thus coherent states are really just harmonic oscillator ground states displaced from the origin[6]. Let us now come the punchline of this class. Given that we have a coherent state how does it time-evolve? We know it is not a stationary state so it must exhibit non-trivial dynamics. In fact it is very straightforward to compute it motion since

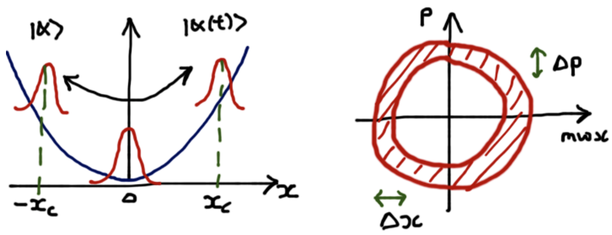
$$\begin{aligned}
e^{-i\hat{H}t/\hbar}\,|\alpha\rangle &= e^{-i(\omega\hat{A}^\dagger\hat{A}+\frac{1}{2}\omega)t}\,|\alpha\rangle\,, \\
&= e^{-i(\omega\hat{n}+\frac{1}{2}\omega)t}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}\,|n\rangle\,, \\
&= e^{-\frac{1}{2}i\omega t}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-i\omega\hat{n}t}\,|n\rangle\,, \\
&= e^{-\frac{1}{2}i\omega t}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}e^{-i\omega nt}\,|n\rangle\,, \\
&= e^{-\frac{1}{2}i\omega t}e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}}\,|n\rangle\,, \\
&= e^{-\frac{1}{2}i\omega t}\left|\alpha e^{-i\omega t}\right\rangle, \\
&= |\alpha(t)\rangle\,.
\end{aligned}$$

Ignoring the irrelevant global phase $e^{-\frac{1}{2}i\omega t}$ arising from the zero-point energy we see that the time-evolution of a coherent state $|\alpha\rangle$ is simply another coherent state defined by a parameter $\alpha(t) = \alpha e^{-i\omega t}$ which differs from α only by a time-varying phase, while its modulus remains constant. As Eq. (4) and Eq. (5) show the phase of the complex parameter defining a coherent state controls its momentum and position. Given we initially have $\alpha = |\alpha|e^{i(\delta_0+\frac{1}{2}\pi)}$ then

$$\begin{aligned}
\langle\alpha(t)|\,\hat{x}\,|\alpha(t)\rangle &= a_{\rm ho}\sqrt{2}\,|\alpha|\sin(\omega t+\delta_0), \\
\langle\alpha(t)|\,\hat{p}\,|\alpha(t)\rangle &= \frac{\hbar}{a_{\rm ho}}\sqrt{2}\,|\alpha|\cos(\omega t+\delta_0),
\end{aligned}$$

from which we identify the initial displacement as $x_0 = a_{\rm ho}\sqrt{2}\,|\alpha|$. This shows that the time dependence of $\langle\hat{x}\rangle$ and $\langle\hat{p}\rangle$ for $|\alpha(t)\rangle$ obey precisely the same equations as a classical harmonic oscillator we considered earlier. However, being quantum mechanical the coherent state does not trace out a perfect circle in phase space, like we drew right back at the start for the classical oscillator. Instead it traces out a "doughnut" with the width given by the minimum uncertainty of the ground state that it retains during its motion.

[6]Mathematically we can link the ground state and coherent state via a unitary $D(\alpha) = \exp(\alpha\hat{A}^\dagger - \alpha^*\hat{A})$ which implements the mapping $|\alpha\rangle = D(\alpha)\,|0\rangle$ and is called a displacement transformation.



The gaussian wave-function of a coherent state therefore does not change shape and instead has a centre whose location oscillates precisely between the classical turning points. Coherent states are therefore the quantum states whose dynamical behaviour most closely resembles our classical intuition of simple harmonic motion.