The Harmonic Oscillator

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1 Introduction

Quantum Theory has many concepts which are counter-intuitive. It is all very well for me to stand here and tell you what is going on, but that doesn't really help counter this problem. There is only one way to overcome this and that is to do the experiment and to solve the equations and then see that the two are in fact in accord.

Unfortunately, we don't have all the sophisticated equipment necessary to do any of the experiments to a degree of accuracy that would satisfy the average physicist, however we can do the calculations. As you are all mathematicians then I just have to hope that you will believe the equations and take it as a given that they agree with the experiments.

The Harmonic Oscillator is a fairly unique type of problem in mathematical physics. It is simple enough to be solved exactly. It involves no major simplification of the physical problem. It is very instructive as to the techniques of Quantum Theory. And finally, if you want to understand anything about Quantum Field Theory then you have to understand the Harmonic Oscillator first since QFT says that all fields are infinite collections of Harmonic Oscillators.

During my undergraduate years, despite being quite definitely a pure mathematician and intending always to be so (except for one horrible year when I went completely off the rails and thought about being a statistician) then I went along to all the lecture courses on Quantum Theory that were on offer. These were titled: Quantum Theory, Further Quantum Theory, Quantum Field Theory. In each of these then we dealt with the Harmonic Oscillator in slightly different ways. What I hope to do is go through these so that you've met them all in regard to a simple problem.

2 The Harmonic Oscillator

Everyone who has done A-Level physics should have heard of the simple harmonic oscillator. It is generally introduced first as the equation of motion of a pendulum oscillating through small angles[1]. It also applies to undamped oscil-

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[1] Small enough that the approximation $\sin\theta = \theta$ is valid.

lations of springs, to plucking a taut string such as on a guitar and many more examples.

We will deal with the one dimensional problem. We have a particle who's position is given by the coordinate x. This coordinate can take any value on the real line. The particle experiences a force towards the origin proportional to the distance from the origin. In Classical mechanics, we have $F = -kx$, where k is some positive constant. Using Newton's second law, we thus have $m\ddot{x} = -kx$.

Now this force can be written as the gradient of a potential. In one dimension, all that means is that it is the derivative of a function. In this case the potential is $V = \frac{1}{2}kx^2$. So we have:

$$m\ddot{x} = -\frac{dV}{dx}$$

The classical solution of this is:

$$x = A\sin\omega t + B\sin\omega t, \quad \omega = \sqrt{\frac{k}{m}}$$

In order to convert to the Quantum problem, we need to identify the momentum and the energy of this particle. The actual method involved uses the Lagrangian and Hamiltonian formulations of Classical Mechanics as the general method. However, you won't be surprised to learn that we have:

$$\begin{aligned} p &= m\dot{x} \\ E &= \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 \\ &= \frac{1}{2m}p^2 + \frac{1}{2}kx^2 \end{aligned}$$

When we quantize this system we use a general method called Dirac Quantization. In this case, all it involves is substituting p by the operator $-i\hbar\frac{d}{dx}$ and x by the operator which multiplies a function by x, i.e. the operator $f(x) \rightarrow xf(x)$.

Schrödinger's equation then becomes:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x}\psi + \frac{1}{2}kx^2\psi = i\hbar\frac{\partial}{\partial t}\psi \tag{1}$$

where ψ is the wave function of the particle so is a function $\psi : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{C}$, where the first coordinate is time and the second space. The interpretation of ψ is that the probability of finding the particle in a section S of the real line at time t is given by:

$$P = \int_S \|\psi(t,x)\|^2 dx$$

Now we need to apply standard differential equation techniques to (1). First we separate ψ into time and space dependent parts by writing $\psi(t,x) = f(t)\phi(x)$. Using this and dividing through by ψ we get:

$$\frac{1}{\phi}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi + \frac{1}{2}kx^2\phi\right) = \frac{1}{f}i\hbar\frac{d}{dt}f \tag{2}$$

The left-hand side is now an equation of space only and the right-hand side of time only. Since space and time are independent variables in our problem, both sides must be equal to some constant which we call E. This constant is the total energy of the particle. Thus:

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi + \frac{1}{2}kx^2\phi &= E\phi && (3) \\ i\hbar\frac{d}{dt}f &= Ef && (4) \end{aligned}$$

The time equation has the simple solution:

$$f(t) \sim e^{-iEt/\hbar}$$

The reason for the proportional sign is that ψ is determined by Schrödinger's equation upto a multiplicative constant. That constant is chosen so that the integral of $\|\psi\|^2$ over the entire real line is 1, i.e. the probability of finding the particle somewhere is 1.

Thus as time progresses, all that happens to the state is that its phase factor rotates at a rate proportional to the constant E.

To solve the space equation, we need more powerful tools. First, we get rid of all the annoying constants by introducing variable ξ and constant λ defined by:

$$\begin{aligned} \xi &= \alpha x, \quad \alpha^4 = \frac{mk}{\hbar^2} = \left(\frac{m\omega}{\hbar}\right)^2 \\ \lambda &= \frac{2E}{\hbar}\sqrt{\frac{m}{k}} = \frac{E}{\frac{1}{2}\hbar\omega} \end{aligned}$$

This simplifies (3) to:

$$\frac{d^2\phi}{d\xi^2} + (\lambda - \xi^2)\phi = 0$$

The asymptotic form of this is:

$$\frac{d^2\phi}{d\xi^2} - \xi^2\phi = 0$$

which looks like it will have solution like $\phi \sim \xi^p e^{\pm\frac{1}{2}\xi^2}$. Since we want a solution that will integrate out to 1 then we must have it converging at infinity, so we try $\phi = H(\xi)e^{-\frac{1}{2}\xi^2}$ and solve for H:

$$\frac{d^2H}{d\xi^2} - 2\xi\frac{dH}{d\xi} + (\lambda - 1)H = 0 \tag{5}$$

This is still not the nicest equation to solve, so we use series solutions. That is, we suppose that H has the form:

$$H(\xi) = \sum_{s=0}^{\infty} a_s \xi^{s+c}, \quad a_0 \neq 0$$

Substituting this in gives a recurrence relation on the a_n:

$$\begin{aligned} a_0c(c-1) &= 0 \\ a_1(c+1)c &= 0 \\ a_{s+2}(s+2)(s+1) &= a_s(2s+1-\lambda) \\ \implies \frac{a_{s+2}}{a_s} &= \frac{2s+1-\lambda}{(s+2)(s+1)} \end{aligned} \tag{6}$$

The first two give us that $c = 0$ and a_0, a_1 are arbitrary constants.

If the series does not terminate, then asymptotically we have:

$$\frac{a_{s+1}}{a_2} \sim \frac{2}{s}.$$

The series expansion for e^{ξ^2} has general term:

$$\frac{1}{\left(\frac{s}{2}\right)!}, \quad s \in 2\mathbb{Z},$$

the common ratio of such terms is:

$$\frac{\left(\frac{s}{2}\right)!}{\left(\frac{s+2}{2}\right)!} = \frac{1}{\frac{s}{2}+1} \sim \frac{2}{s}$$

So if the series for H doesn't terminate, it behaves asymptotically like e^{ξ^2}. This means that the final solution for ϕ would behave like $e^{\frac{1}{2}\xi^2}$, which is not a valid solution. Thus the series must terminate.

If the n^{th} term is the last non-zero term, then using (6) we find that $\lambda = 2n + 1$.

For each value of n we get a different polynomial, H_n, called the n^{th} *Hermite Polynomial*. They are alternatively odd and even functions of ξ. Each is a solution of the differential equation (5) and so each gives a solution to the space equation. Thus we have a family of solutions parameterized by the positive integers:

$$\phi_n(\xi) = N_n e^{-\frac{1}{2}\xi^2} H_n(\xi)$$

where N_n is a normalizing constant. The energy of each solution is:

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

Notice that the lowest solution, corresponding to $n = 0$, still has positive energy $\frac{1}{2}\hbar\omega$.

Thus the complete solution to the Harmonic Oscillator is:

$$\psi = \sum_{n=0}^{\infty} c_n \psi_n \tag{7}$$

where:

$$\begin{aligned}
\psi_n &= N_n e^{-\frac{1}{2}\alpha x^2} H_n(\alpha x) e^{-iE_n t/\hbar} \\
E_n &= (n + \frac{1}{2})\hbar\omega \\
\sum_{n=0}^{\infty} |c_n|^2 &= 1
\end{aligned}$$

The states ψ_n form an orthonormal basis in our Hilbert space of states and are called the *Normal Modes* of the Harmonic Oscillator.

It is worth taking a moment to consider what we have actually calculated. We knew from the outset, through general theory, that the Hilbert space of instantaneous states would be $L^2(\mathbb{R}, \mathbb{C})$. What we know now is how a state evolves in time. All we need to do is express it as a linear combination of normal modes. These normal modes then have a particularly simple time evolution.

Remember, though, that states contain information about *probabilities.* The probability that the particle will be found in a certain region is found by squaring the absolute value of the state and integrating over that region. It may be useful to look at the graphs of $\|\psi(t, x)\|^2$.

First for $\|\psi_0(t, x)\|^2$. The graph of this is in figure 1. This state does not appear to evolve in time. It appears to be a static bell-shaped curve centred at the origin.

The graph for $\|\psi_1(t, x)\|^2$, in figure 2, also seems static. This time there is a dip in the graph at the origin, so that if the particle is in this mode, it is impossible to find it at the origin[2].

It is not until you consider a mixed state, as in figure 3, that the true picture starts to emerge. Consider a state which is half ψ_0 and half ψ_1. Thus whenever one measures the energy of this state, it is E_0 or E_1 with equal probability. This state really does evolve in time. Notice that the hump does not oscillate back and forth, but spreads out and then re-forms in a different place. But note that if you measure the energy, and thus force it into one or the other state, then whatever time it is it always has equal probability of being in either state.

What we have also calculated is the energy eigenstates and eigenvalues. Recall that given a self-adjoint operator we can do two things with it. We can either directly observe it or we can calculate the expected value of observing it. In the first case we disturb the system and force it into an eigenstate and our measurement is an eigenvalue of the operator. One thing to notice is that we have a genuine observable operator with discrete spectrum. That means that whenever we observe the energy of the Harmonic Oscillator, what we measure is of value $(n + \frac{1}{2})\hbar\omega$ for some n.

Suppose we are in the state given by (7). Then the expected value of the

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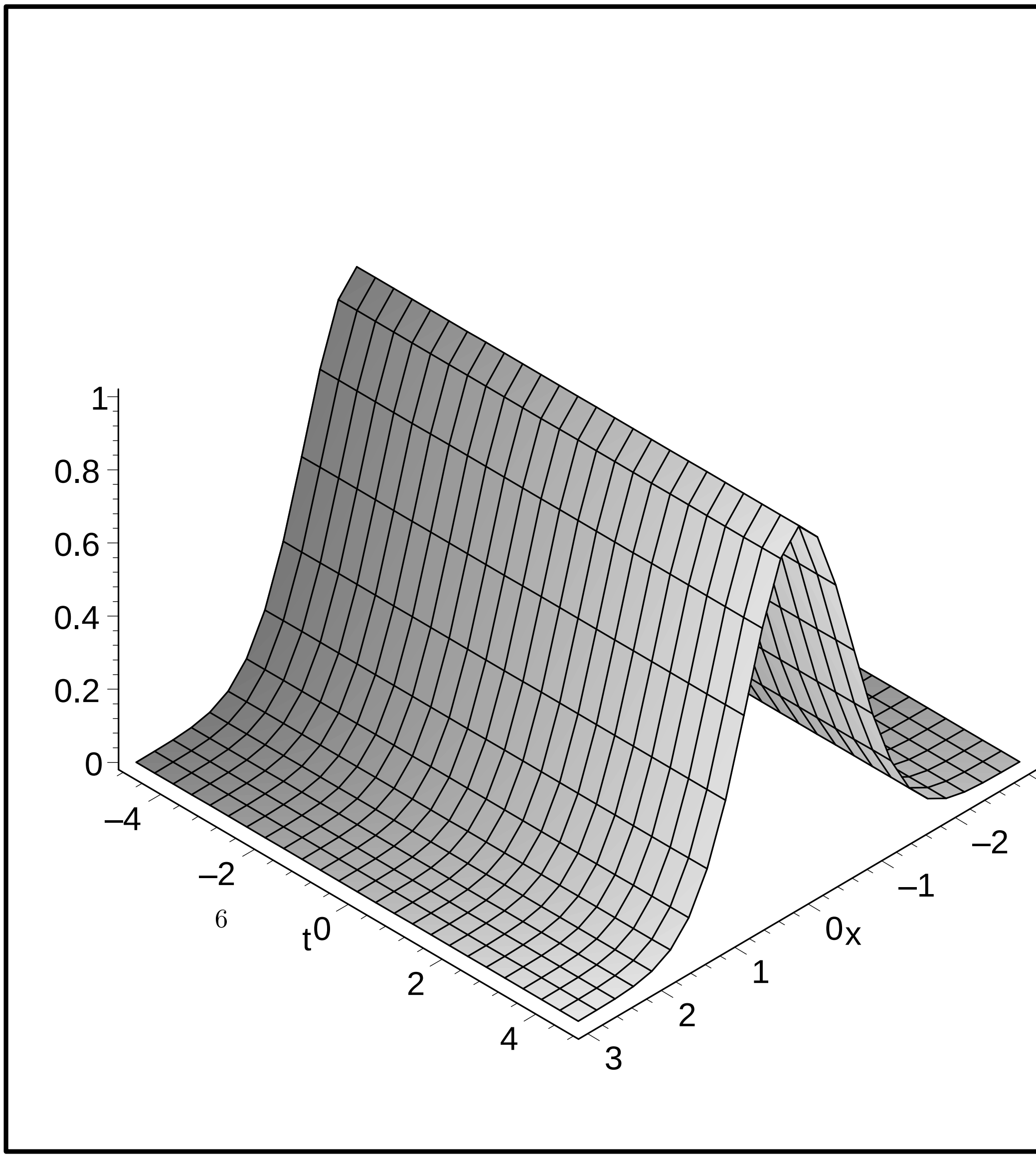
[2] In practice, however, since the apparatus used must be of a finite size, the best one can do is to find it *near* the origin - an event which does have a non-zero probability.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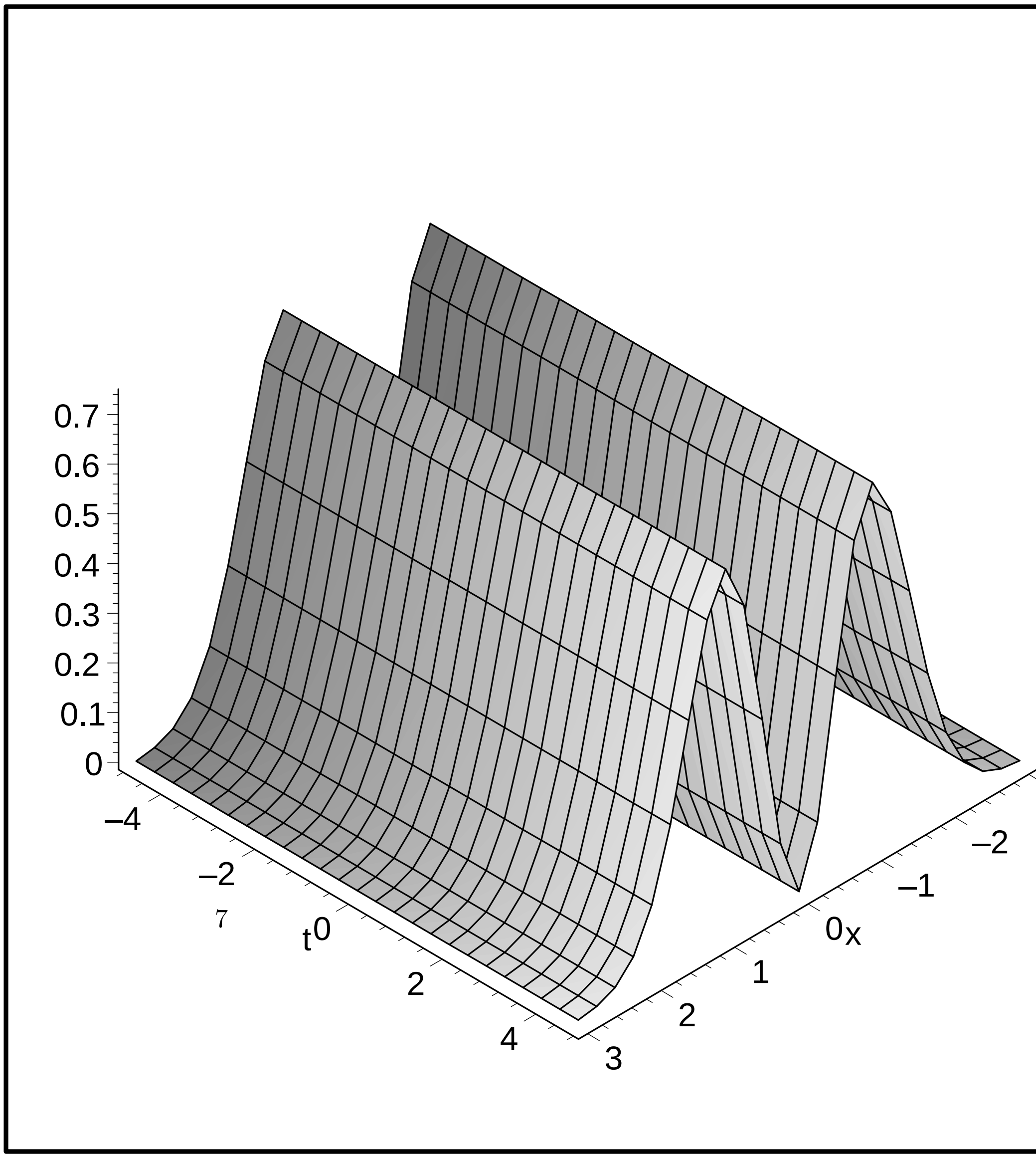
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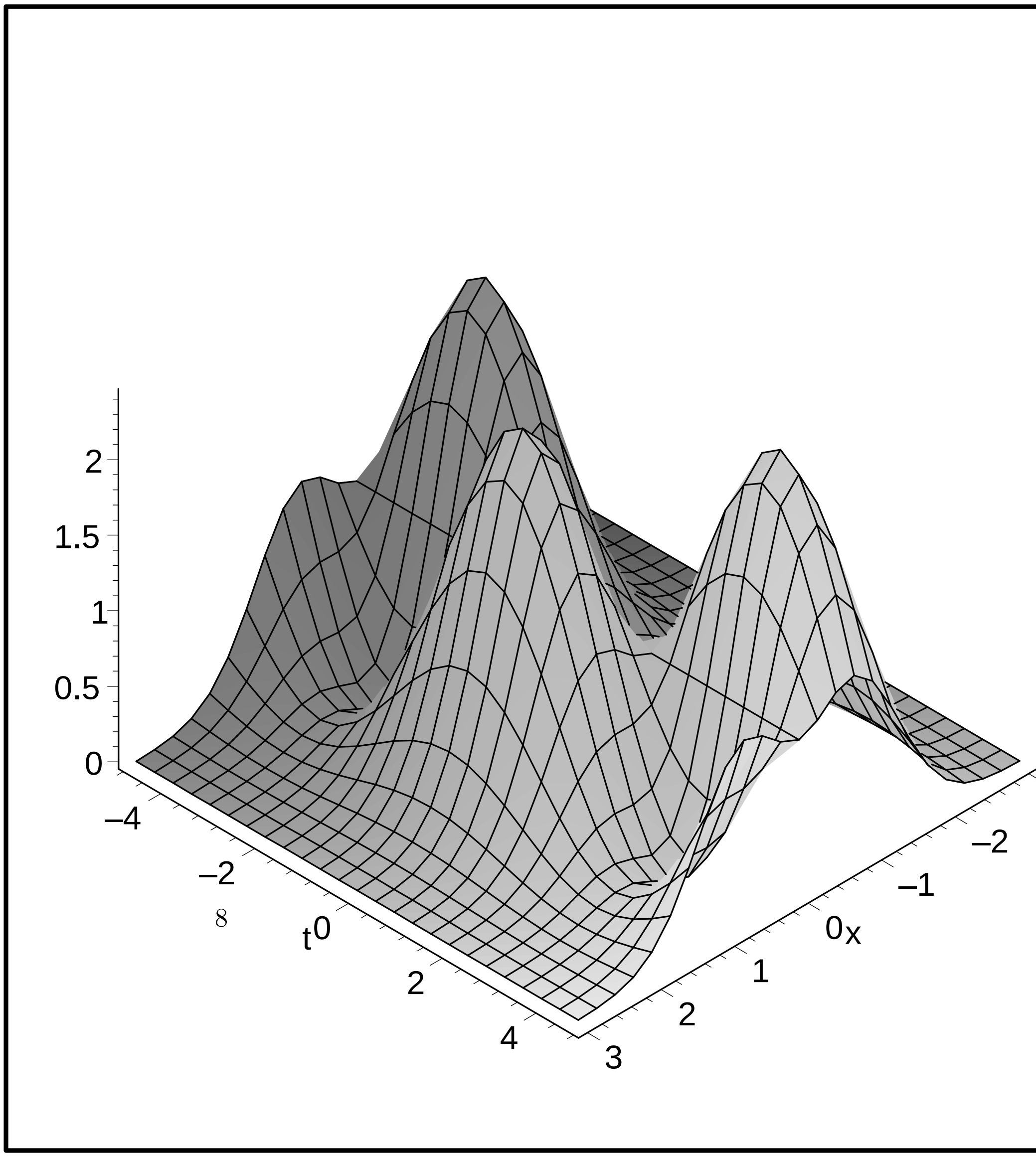
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energy is:

$$\begin{aligned}\langle\psi|E|\psi\rangle &= \sum_{n=0}^{\infty}|c_n|^2E_n\\ &= \sum_{n=0}^{\infty}|c_n|^2(n+\frac{1}{2})\hbar\omega\end{aligned}$$

and the effect of actually observing the energy is to force ψ into the eigenstate ψ_n with probability $|c_n|^2$.

3 Creation and Annihilation

The Harmonic Oscillator Hamiltonian is given by:

$$H = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2X^2$$

where we have eliminated k from the equation. Here we are using the notation of P for the momentum operator and X for the position operator. Thus:

$$P\psi(x) = -i\hbar\frac{d\psi}{dx}(x) \quad X\psi(x) = x\psi(x)$$

Consider the commutator of the momentum and position operators. So that we don't get confused with the operator which multiplies by x and the variable x, we shall apply these to an arbitrary state, ψ:

$$\begin{aligned}[P,X]\,\psi(x) &= -i\hbar\frac{d}{dx}x\psi(x) - x\left(-i\hbar\frac{d}{dx}\psi(x)\right)\\ &= -i\hbar\left(\psi(x) + x\frac{d\psi}{dx}(x) - x\frac{d\psi}{dx}(x)\right)\\ &= -i\hbar\psi(x)\end{aligned}$$

Hence:

$$[P,X] = -i\hbar I$$

Let $A = \frac{1}{\sqrt{2m\omega}}(P - im\omega X)$ and let A^* be the complex conjugate of A.

Then we have the following identities:

$$\begin{aligned} AA^* &= \frac{1}{2m\omega}\left(P^2 + m^2\omega^2 X^2 + im\omega\,[P,X]\right) \\ &= \frac{1}{\omega}\left(H + \frac{1}{2}\hbar\omega\right) \\ A^*A &= \frac{1}{\omega}\left(H - \frac{1}{2}\hbar\omega\right) \\ \text{So: } [A,A^*] &= \hbar\omega \\ \text{And: } H &= \omega AA^* - \frac{1}{2}\hbar\omega \\ &= \omega A^*A + \frac{1}{2}\hbar\omega \end{aligned}$$

Using these, we get:

$$AH - HA = \hbar\omega A \tag{8}$$

$$A^*H - HA^* = \hbar\omega A^* \tag{9}$$

Now the Hamiltonian operator measures the energy of the system. Suppose that ψ is an energy eigenstate with eigenvalue E. Then applying (8) and (9) to ψ gives:

$$\begin{aligned} HA\psi &= (E - \hbar\omega)A\psi \\ HA^*\psi &= (E + \hbar\omega)A^*\psi \end{aligned}$$

so provided they are non-zero, $A\psi$ and $A^*\psi$ are also eigenstate of H with eigenvalues $E - \hbar\omega$ and $E + \hbar\omega$ respectively.

Consider the norm of $A\psi$ with ψ itself normalized:

$$\begin{aligned} \|A\psi\|^2 &= \langle A\psi|A\psi\rangle \\ &= \langle A^*A\psi|\psi\rangle \\ &= \frac{1}{\omega}\left[\langle\psi|H\psi\rangle - \frac{1}{2}\hbar\omega\|\psi\|^2\right] \\ &= \frac{1}{\omega}\left(E - \frac{1}{2}\hbar\omega\right) \\ \text{Thus: } E &= \frac{1}{2}\hbar\omega + \omega\|A\psi\|^2 \\ &\geq \frac{1}{2}\hbar\omega > 0 \end{aligned}$$

Thus the energy is always positive. Now applying A to an eigenstate of H lowers the eigenvalue by $\hbar\omega$. Since the energy is always positive, this must eventually stop. It can only stop when $A\psi = 0$, which occurs when $E = \frac{1}{2}\hbar\omega$.

Then looking at the norm of $A^*\psi$ we see that:

$$\|A^*\psi\|^2 = \frac{1}{\omega}E + \frac{1}{2}\hbar$$

and this is always positive since E is always positive.

Thus A^* always takes us from one eigenstate to another with higher energy level.

Our conclusions from all of this are as follows. Consider the null space of A. If this is non-null, we call states in this space *vacuum states*. Then eigenstates of H are given by the formula ${A^*}^n\Phi$ (renormalized) with eigenvalue $(n+\frac{1}{2})\hbar\omega$.

Now consider the operator $\frac{1}{\hbar}A^*A$. This is self-adjoint and so is an observable. Since it is just a multiple of H plus a multiple of the identity, it's eigenstates are just those of H. It's action is given by:

$$A^*A\,({A^*}^n\Phi) = n\,({A^*}^n\Phi)$$

So this operator "counts" how far from the vacuum state one is. It is called the *number operator*.

The operators A and A^* are called the *annihilation* and *creation* operators respectively. The annihilation operator corresponds to the system losing energy and the creation to it gaining energy. For our purposes, we have been considering a closed system which cannot gain or lose energy and so all they do is allow us to obtain the energy eigenstates.

The vacuum states are also called *ground states* and the other states are called *excited states*.