9 Quantum harmonic oscillators

This part of the course is essentially a brief revision of you have seen in the Michaelmas Term, with an extention to 3D oscillators. Harmonic oscillators are of great importance in Classical Mechanics, not the least because the motion of systems of particles in the vicinity of a configuration of stable equilibrium can often be described in terms of coupled harmonic oscillators. This is also the case in Quantum Mechanics.

9.1 The Hamiltonian and the energy levels of a linear harmonic oscillator

In Classical Mechanics, a linear harmonic oscillator is a mass point subject to a force $\mathbf{F}$ proportional to its displacement from a fixed point and constrained to move along a straight line (here taken to be the x-axis): $\mathbf{F} = -k(x - x_0)\,\hat{x}$, where x is the position of the mass, x_0 is its equilibrium position, k is the "spring constant", and $\hat{x}$ is a unit vector in the positive x-direction. In Hamiltonian Mechanics, this system is described by a Hamiltonian function $H(p, x)$, where p (the canonical momentum) is the generalized momentum conjugate to the co-ordinate x. Here $p = m\mathrm{d}x/\mathrm{d}t$, with m the mass of the oscillator, and

$$H(p, x) = \frac{p^2}{2m} + \frac{1}{2}\,k\,x^2. \tag{9.1}$$

The corresponding equations of motion are solved readily: The mass point describes a harmonic oscillation at an angular frequency ω related to the spring constant k and the mass m by the equation $\omega = (k/m)^{1/2}$. (A "harmonic oscillation" is an oscillation described by a sine or cosine function.) Making use of this relation, Eq. (9.1) can be recast as

$$H(p, x) = \frac{p^2}{2m} + \frac{1}{2}\,m\omega^2 x^2. \tag{9.2}$$

The corresponding quantum mechanical Hamiltonian is obtained from the classical Hamiltonian by replacing p by the momentum operator $\hat{p}_x$ and x by the position operator $\hat{x}$:

$$H(p, x) \to \hat{H} = \frac{1}{2m}\hat{p}_x^2 + \frac{1}{2}\,m\omega^2\,\hat{x}^2. \tag{9.3}$$

In the position representation, the operators $\hat{x}$ and $\hat{p}_x$ are taken to be the operators which transform a wave function $\Psi(x, t)$ into, respectively, $x\Psi(x, t)$ and

$-i\hbar \mathrm{d}\Psi/\mathrm{d}x$, with the result that $\hat{H}$ is then represented by the following operator, which we have already seen several times:

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}\,m\omega^2 x^2. \tag{9.4}$$

It turns out that the time-independent Schrödinger equation can be solved exactly for this Hamiltonian, either as a differential equation or by using algebraic methods based on the ladder operator mentioned in the next section. The following is found:

1. The eigenenergies of the linear Harmonic oscillator and the corresponding energy eigenstates can be labelled by an integer n which can take any non-negative value:

   $$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle, \quad n = 0, 1, 2, \ldots, \tag{9.5}$$

   or in the position representation,

   $$H\psi_n(x) = E_n\psi_n(x), \quad n = 0, 1, 2, \ldots \tag{9.6}$$

2. Each of the eigenenergies E_n is non degenerate, and

   $$E_n = \hbar\omega(n + 1/2). \tag{9.7}$$

   These eigenenergies thus form a ladder of equally spaced energy levels. The bottom "rung" — i.e., the ground state energy — is $E_0 = \hbar\omega/2$, and each level is separated from the adjacent levels by an energy $\hbar\omega$. (Note that the ground state energy is non-zero.)

9.2 The ladder operators

The ladder operators for a linear harmonic oscillator were introduced in the Term 1 QM course. These operators were denoted by a_- and a_+ in that course and were defined in the position representation, in terms of the operators x and $p_x \equiv -i\hbar \mathrm{d}/\mathrm{d}x$. It is convenient to denote the corresponding operators acting on ket vectors by, respectively, $\hat{a}$ (corresponding to a_-) and $\hat{a}^\dagger$ (the adjoint of $\hat{a}$, corresponding to a_+). These two operators have the important property of satisfying the following commutation relation:

$$[\hat{a}, \hat{a}^\dagger] = 1. \tag{9.8}$$

Moreover, the Hamiltonian of a linear harmonic oscillator of angular frequency ω can be written in terms of the operators $\hat{a}$ and $\hat{a}^\dagger$ as

$$\hat{H} = \hbar\omega\big(\hat{a}^\dagger\hat{a} + 1/2\big). \tag{9.9}$$

Note that this Hamiltonian is exactly the same as the Hamiltonian $\hat{H}$ of Eq. (9.3); the only difference is that $\hat{H}$ is now written in terms of the operators $\hat{a}$ and $\hat{a}^\dagger$ instead of the operators $\hat{x}$ and $\hat{p}_x$.

☞ How these two operators came about is easily understood by noting that Eq. (9.2) can also be written as

$$H(p,x) = \left(\sqrt{\frac{m\omega^2}{2}}\,x + i\sqrt{\frac{1}{2m}}\,p\right)\left(\sqrt{\frac{m\omega^2}{2}}\,x - i\sqrt{\frac{1}{2m}}\,p\right), \quad (9.10)$$

or as $H(p,x) = A^*A$ with

$$A = \sqrt{\frac{m\omega^2}{2}}\,x + i\sqrt{\frac{1}{2m}}\,p. \quad (9.11)$$

Passing to the quantum mechanical Hamiltonian is then done by setting $a = A/\sqrt{\hbar\omega}$, writing $H(p,x)$ as $\hbar\omega(aa^* + a^*a)/2$, and replacing a by the operators $\hat{a}$ and a^* by the adjoint of $\hat{a}$ with

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + i\sqrt{\frac{1}{2m\hbar\omega}}\,\hat{p}, \qquad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - i\sqrt{\frac{1}{2m\hbar\omega}}\,\hat{p}. \quad (9.12)$$

A and A^* were divided by $\sqrt{\hbar\omega}$ in the above so as to make the corresponding operators $\hat{a}$ and $\hat{a}^\dagger$ dimensionless. Since $a^*a \equiv aa^*$, $\hbar\omega(aa^* + a^*a)/2 \equiv \hbar\omega a^*a$. However, $\hbar\omega(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger)/2 \neq \hbar\omega\hat{a}^\dagger\hat{a}$ since $\hat{a}^\dagger\hat{a} \neq \hat{a}\hat{a}^\dagger$. Replacing a and a^* by $\hat{a}$ and $\hat{a}^\dagger$ in $\hbar\omega(aa^* + a^*a)/2$ rather than in $\hbar\omega a^*a$ ensures that the correct quantum mechanical Hamiltonian is obtained. (Note that $\hbar\omega(\hat{a}^\dagger\hat{a} + \hat{a}\hat{a}^\dagger)/2 = \hbar\omega(\hat{a}^\dagger\hat{a} + 1/2)$ since $\hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1$.)

As was shown in the term 1 QM course, the energy levels E_n can be deduced from Eq. (9.9) and from the commutation relation of $\hat{a}$ and $\hat{a}^\dagger$ by a purely algebraic method (i.e., without solving the Schrödinger equation as a differential equation). A key result from this approach is that it is possible to find a set of normalized energy eigenstates $\{|\psi_n\rangle, n = 0, 1, \ldots\}$ such that

$$\hat{a}|\psi_n\rangle = \sqrt{n}|\psi_{n-1}\rangle \quad \text{with} \quad \hat{a}|\psi_0\rangle = 0, \quad (9.13)$$

$$\hat{a}^\dagger|\psi_n\rangle = \sqrt{n+1}|\psi_{n+1}\rangle. \quad (9.14)$$

A number of other results can be derived from this, e.g., that $\hat{n} = \hat{a}^\dagger\hat{a}$ is a number operator:

$$\hat{n}|\psi_n\rangle = n|\psi_n\rangle, \quad (9.15)$$

and also that $\hat{H}|\psi_n\rangle = \hbar\omega(n + 1/2)|\psi_n\rangle$. Going up from the energy level E_n to the one immediately above amounts to adding a "quantum of energy" $\hbar\omega$

to E_n. Compared to the ground state $|\psi_0\rangle$, the energy eigenstate $|\psi_n\rangle$ can be understood as containing n quanta of energy. The operator $\hat{n}$ thus "counts" the number of energy quanta contained in the states it acts on.

☞ Iterating Eq. (9.14) gives all the normalized energy eigenstates $|\psi_n\rangle$ in terms of the ground state, $|\psi_0\rangle$:

$$|\psi_n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n |\psi_0\rangle. \tag{9.16}$$

Because these various properties hold irrespective of whether the Schrödinger equation can or cannot be written as a differential equation, they carry over to systems which cannot be formulated in the position representation — e.g., to photon fields in quantum electrodynamics. Similar ladder operators are also widely used in quantum field theory. You may also remember that the eigenvalues of angular momentum operators can be derived algebraically using ladder operators.

Extension to 3D

Similar ladder operators can be introduced for 3D harmonic oscillators. namely $\hat{a}_x$ and $\hat{a}_x^\dagger$ (the same as $\hat{a}$ and $\hat{a}^\dagger$) and also $\hat{a}_y$, $\hat{a}_y^\dagger$, $\hat{a}_z$ and $\hat{a}_z^\dagger$. The operators $\hat{a}_y$ and $\hat{a}_z$ and their adjoints are related to the position operators $\hat{y}$ and $\hat{z}$ and to the momentum operators $\hat{p}_y$ and $\hat{p}_z$ in the same way as $\hat{a}_x$ and $\hat{a}_x^\dagger$ are related to $\hat{x}$ and $\hat{p}_x$. These operators are such that

$$[\hat{a}_x, \hat{a}_x^\dagger] = [\hat{a}_y, \hat{a}_y^\dagger] = [\hat{a}_z, \hat{a}_z^\dagger] = 1. \tag{9.17}$$

Recall that position and momentum operators pertaining to orthogonal directions always commute with each other, and also that position operators always commute with other position operators and momentum operators always commute with other momentum operators. Therefore ladder operators pertaining to orthogonal directions also commute with each other. In particular,

$$[\hat{a}_x, \hat{a}_y^\dagger] = [\hat{a}_x, \hat{a}_z^\dagger] = 0, \tag{9.18}$$
$$[\hat{a}_y, \hat{a}_x^\dagger] = [\hat{a}_y, \hat{a}_z^\dagger] = 0, \tag{9.19}$$
$$[\hat{a}_z, \hat{a}_x^\dagger] = [\hat{a}_z, \hat{a}_y^\dagger] = 0. \tag{9.20}$$

9.3 The coherent states of a simple harmonic oscillator

As you may remember from a previous Quantum Mechanics course, the wave function $\Psi(\mathbf{r}, t)$ describing the quantum state of a free particle can always be written as a superposition of plane waves — i.e., as an integral of the form

$$\Psi(\mathbf{r}, t) = \frac{1}{(2\pi)^{3/2}} \int \phi(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}) \exp(-iE_k t/\hbar)\, \mathrm{d}^3 k, \tag{9.21}$$

where $E_k = \hbar^2 k^2/2m$ and $\phi(\mathbf{k})$ is a certain function of the wave vector $\mathbf{k}$. (We stress that this result applies to the case of a *free* particle, namely a particle not interacting with anything. The potential energy of a free particle is the same everywhere in space and at all times, and can be taken to be identically zero by choice of the origin of the energy scale.) How the probability density $|\Psi(\mathbf{r}, t)|^2$ varies with $\mathbf{r}$ and t depends on the function $\phi(\mathbf{k})$, and so does the uncertainty Δx on the position of this particle. However, whatever $\phi(\mathbf{k})$ is, it is always the case that Δx will increase without limit as $t \to \infty$: a free particle always become more and more delocalized at large times. This delocalization is often referred to as the spreading of the wave packet.

Remarkably, non-spreading wave functions are possible for the case of a particle trapped in a quadratic potential well (i.e., if the particle is a simple harmonic oscillator). I.e, when the Hamiltonian is given by Eq. (9.4), the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi(x, t) \tag{9.22}$$

has solutions for which Δx remains constant in time. These wave functions describe a particular class of states called coherent states (the word "coherent" meaning that the wave packet "coheres", i.e., remains together rather than spreads out). Here is a list of interesting facts about coherent states (see the homework and workshop problems associated with the course for proofs of many these results):

1. The coherent states are the eigenstates of the ladder operator $\hat{a}$. Any real or complex number α is an eigenvalue of $\hat{a}$ and the coherent states are described by the corresponding eigenvectors: If

   $$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \tag{9.23}$$

   then $|\alpha\rangle$ describes a coherent state. (In contrast, the operator $\hat{a}^\dagger$ has no eigenvector.)

2. The symbol $|\alpha\rangle$ is usually reserved for the normalized eigenvectors of $\hat{a}$. The coherent state $|0\rangle$ corresponding to $\alpha = 0$ is the ground state

of the oscillator. (I.e., $|0\rangle = |\psi_0\rangle$ in the notation used above.) Coherent states other than $|0\rangle$ are not eigenstates of the Hamiltonian. Hence they depend on time (when one works in the so-called Schrödinger representation, see Part 11 of these notes). Within an overall constant factor,

$$|\alpha\rangle(t) = \exp(-|\alpha|^2/2) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \exp(-iE_n t/\hbar)|\psi_n\rangle, \tag{9.24}$$

where the energies E_n and the energy eigenstates $|\psi_n\rangle$ are defined as in Eqs. (9.7) and (9.16).

3. The expectation values of the position and of the momentum vary in time like the position and the momentum of a simple harmonic oscillator in classical mechanics. Specifically, in a state $|\alpha\rangle$,

$$\langle x\rangle(t) = 2|\alpha|\sqrt{\frac{\hbar}{2m\omega}}\,\cos(\omega t - \arg\alpha), \tag{9.25}$$

$$\langle p\rangle(t) = -2|\alpha|\sqrt{\frac{m\hbar\omega}{2}}\,\sin(\omega t - \arg\alpha). \tag{9.26}$$

The modulus and the argument of the complex number α thus define the amplitude and the phase of the oscillation.

4. Defining uncertainties as in Section 6.4, the uncertainties on the position and on the momentum of a particle in a coherent state $|\alpha\rangle$ are given by the following equations:

$$\Delta x = \sqrt{\frac{\hbar}{2m\omega}}, \qquad \Delta p = \sqrt{\frac{m\hbar\omega}{2}}. \tag{9.27}$$

These uncertainties are constant in time (the wave packet does not spread) and are the same for any coherent state (they do not depend on α). Moreover, their product takes on the lowest value allowed by the Heisenberg uncertainty principle:

$$\Delta x \Delta p = \hbar/2. \tag{9.28}$$

5. In position representation, $|\alpha\rangle(t = 0)$ can be represented by the wave function

$$\phi_\alpha(x) = C \exp\left(-\left[\sqrt{\frac{m\omega}{2\hbar}}\,x - \alpha\right]^2\right), \tag{9.29}$$

where C is a normalization constant. Since $\phi_\alpha(x)$ is the ground state wave function when $\alpha = 0$, a coherent state can be described as a "displaced ground state".