8 The harmonic oscillator

Contrary to the previously studied piecewise constant potentials that constitute rather crude approximations of the physical reality, one encounters harmonic oscillators everywhere. In classical mechanics, whenever one has an equilibrium configuration at some x_0 , characterised by the minimum of a potential, studying small fluctuations around this minimum involves Taylor expanding the potential V(x) around the minimum, and then $V(x) = V(x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 + \ldots$, where the terms $+ \ldots$ can be neglected as long as $x-x_0$ is small enough, i.e. as long as one only considers small fluctuations. In particular, the vibrational spectra of molecules correspond to harmonic oscillators in a very good approximation. On the other hand, the harmonic oscillator constitutes a quantum mechanical system that can be solved exactly (by which we mean that we can determine all eigenvalues and eigenfunctions exactly). There are not many systems for which this is the case. It is thus worth studying the quantum mechanical harmonic oscillator in some detail. Moreover, there is a very elegant formalism of so-called creation and annihilation operators, and this formalism also plays a very important role in what is called (misleadingly) "second quantisation", as well as in quantum field theory.

8.1 The Hamiltonian and operators a and a^{\dagger}

The classical equations of motion in a (one-dimensional) harmonic potential can be written as

$$\frac{dx_{\rm cl}(t)}{dt} = \frac{p_{\rm cl}(t)}{m} \quad , \quad \frac{dp_{\rm cl}(t)}{dt} = -V'(x_{\rm cl}(t)) \quad , \quad V(x) = \frac{m}{2}\omega^2 x^2 \; , \tag{8.1}$$

which lead, of course, to $\frac{d^2}{dt^2}x_{\rm cl}(t) + \omega^2x_{\rm cl}(t) = 0$ with solutions $x_{\rm cl}(t) = x_0\cos(\omega t + \delta)$. Recall Ehrenfest's relations (6.92) for the expectation values, $\frac{d}{dt}\langle X\rangle = \frac{\langle P\rangle}{m}$ and $\frac{d}{dt}\langle P\rangle = -\langle V'(X)\rangle$. For the (classical) harmonic potential V(x), the first derivative $V'(x) = m\omega^2x$ is linear, and then if we assume that the quantum mechanical hamiltonian also is

$$H = \frac{P^2}{2m} + \frac{m}{2}\omega^2 X^2 \ , \tag{8.2}$$

then $V'(X) = m\omega^2 X$ is linear and we have $\langle V'(X) \rangle = V'(\langle X \rangle)$. Then Ehrenfest's relations for $\langle X \rangle$ and $\langle P \rangle$ are exactly the same equations as the classical equations of motion for $x_{\rm cl}(t)$ and $p_{\rm cl}(t)$. This is a good argument to take (8.2) as the appropriate Hamiltonian for the quantum mechanical harmonic oscillator.³⁸ We will determine the eigenvalues (energy levels) of this Hamiltonian, and find that they are in good agreement with the vibrational spectra of diatomic molecules (with the appropriate values of m and ω). We take this as another, experimental evidence that (8.2) is the appropriate Hamiltonian.

³⁸Of course, in general, for non-quadratic potentials one does not have this exact equality but one nevertheless assumes that the Hamiltonian is given by $\frac{P^2}{2m} + V(X)$.

The eigenvalue problem for H is (recall the relations $\varphi_n(x) = \langle x | \varphi_n \rangle$, as well as $x \varphi_n(x) = \langle x | X | \varphi_n \rangle$ and $-i\hbar \frac{\mathrm{d}}{\mathrm{d}x} \varphi_n(x) = \langle x | P | \varphi_n \rangle$)

$$\left(\frac{P^2}{2m} + \frac{m}{2}\omega^2 X^2\right) |\varphi_n\rangle = E_n |\varphi_n\rangle \quad \Leftrightarrow \quad -\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \varphi_n(x) + \frac{m}{2}\omega^2 x^2 \varphi_n(x) = E_n \varphi_n(x) \ . \tag{8.3}$$

We may proceed in either of the two following ways. We may solve the differential equation for $\varphi_n(x)$ with the boundary conditions that $\varphi_n(x) \to 0$ sufficiently rapidly as $|x| \to \infty$ so that $\varphi_n \in L^2(\mathbb{R})$. This will eventually determine the allowed values of E_n , and then the corresponding eigenfunctions $\varphi_n(x)$. Alternatively, we may use a more algebraic approach which makes use of the commutation relations of X and P, as well as of the positivity of the norm on our Hilbert space. Both approaches are equivalent, since the commutation relation $[X, P] = i\hbar \mathbf{1}$ is of course used in the differential equation since P has translated to $-i\hbar \frac{d}{dx}$, and the positivity of the norm is the requirement that we can obtain a normalisable eigenstate which is the same as asking that $\varphi_n \in L^2(\mathbf{R})$. Since in the previous section we have already much used the method based on solving the differential equation, we now opt for the algebraic approach.

First, let's do some dimensional analysis. Looking at (8.3) we see that $\frac{\hbar^2}{mx^2}$ and $m\omega^2x^2$ have the same dimension (unit), so that $\frac{\hbar}{m\omega}$ must be a length squared and then

$$\gamma = \sqrt{\frac{\hbar}{m\omega}} \tag{8.4}$$

is a characteristic length. Also $\frac{X}{\gamma}$ and $\frac{\gamma}{\hbar}P$ are dimensionless operators. We then introduce the complex combinations

$$a = \frac{1}{\sqrt{2}} \left(\frac{1}{\gamma} X + i \frac{\gamma}{\hbar} P \right) \quad \Leftrightarrow \quad a^{\dagger} = \frac{1}{\sqrt{2}} \left(\frac{1}{\gamma} X - i \frac{\gamma}{\hbar} P \right) . \tag{8.5}$$

Of course, this can be inverted as

$$X = \frac{\gamma}{\sqrt{2}}(a+a^{\dagger}) \quad , \quad P = \frac{\hbar}{\sqrt{2\gamma}i}(a-a^{\dagger}) . \tag{8.6}$$

Let us compute the commutator of a and a^{\dagger} :

$$[a, a^{\dagger}] = \left[\frac{1}{\sqrt{2}\gamma}X, -i\frac{\gamma}{\sqrt{2}\hbar}P\right] + \left[i\frac{\gamma}{\sqrt{2}\hbar}P, \frac{1}{\sqrt{2}\gamma}X\right] = -i\frac{1}{2\hbar}[X, P] + i\frac{1}{2\hbar}[P, X] \tag{8.7}$$

The commutation relations $[X, P] = i\hbar \mathbf{1}$ (and of course $[P, X] = -i\hbar \mathbf{1}$) then translate into

$$[a, a^{\dagger}] = \mathbf{1} . \tag{8.8}$$

We want to express the Hamiltonian in terms of these a and a^{\dagger} . We have

$$\frac{m}{2}\omega^2 X^2 = \frac{1}{4}m\omega^2 \gamma^2 (a + a^{\dagger})^2 = \frac{\hbar\omega}{4} (aa + aa^{\dagger} + a^{\dagger}a + a^{\dagger}a^{\dagger}) . \tag{8.9}$$

Note that $aa^{\dagger} + a^{\dagger}a$ is neither $2aa^{\dagger}$ nor $2a^{\dagger}a$ since the operators do not commute. But we may use the commutator to switch the order by writing

$$aa^{\dagger} = (aa^{\dagger} - a^{\dagger}a) + a^{\dagger}a = [a, a^{\dagger}] + a^{\dagger}a = \mathbf{1} + a^{\dagger}a$$
 (8.10)

This allows us to rewrite (8.9) as

$$\frac{m}{2}\omega^2 X^2 = \frac{\hbar\omega}{4} (aa + 2a^{\dagger}a + a^{\dagger}a^{\dagger} + \mathbf{1}) . \tag{8.11}$$

Similarly

$$\frac{1}{2m}P^2 = \frac{\hbar\omega}{4}(-aa + 2a^{\dagger}a - a^{\dagger}a^{\dagger} + \mathbf{1})$$
 (8.12)

Adding two two previous expressions we get the Hamiltonian (8.2) as

$$H = \hbar\omega(a^{\dagger}a + \frac{1}{2}) , \qquad (8.13)$$

where $+\frac{1}{2}$ really means $+\frac{1}{2}$ 1. We also introduce the (hermitian) operator

$$N = a^{\dagger} a {,} {(8.14)}$$

so that the Hamiltonian can also be written as

$$H = \hbar\omega(N + \frac{1}{2}) \ . \tag{8.15}$$

From the commutation relations of the a and a^{\dagger} one easily finds (recall [A, B] = -[B, A])

$$[N, a] = Na - aN = a^{\dagger}aa - aa^{\dagger}a = (a^{\dagger}a - aa^{\dagger})a = [a^{\dagger}, a]a = -a , \qquad (8.16)$$

and similarly

$$[N, a^{\dagger}] = Na^{\dagger} - a^{\dagger}N = a^{\dagger}aa^{\dagger} - a^{\dagger}a^{\dagger}a = a^{\dagger}(aa^{\dagger} - a^{\dagger}a) = a^{\dagger}[a, a^{\dagger}] = a^{\dagger}. \tag{8.17}$$

(This also follows more easily from taking the hermitian conjugate of (8.16).) These two relations can be rewritten as

$$Na = a(N-1)$$
 , $Na^{\dagger} = a^{\dagger}(N+1)$. (8.18)

Since N is hermitian, it has real eigenvalues which we call n. Moreover, since $H = \hbar\omega(N + \frac{1}{2})$ we see that H and N have the same eigenvectors and that the eigenvalues are related by $E_n = \hbar\omega(n + \frac{1}{2})$. We now want to establish that the eigenvalues n are non-negative integers. Let $N |n\rangle = n |n\rangle$. It follows that

$$N(a|n\rangle) = a(N-1)|n\rangle = a(n-1)|n\rangle = (n-1)(a|n\rangle),$$
 (8.19)

so that $a|n\rangle$, if non-vanishing, is another eigenvector of N with eigenvalue n-1. We say that a lowers the eigenvalue by one unit. Similarly

$$N(a^{\dagger} | n \rangle) = a^{\dagger} (N+1) | n \rangle = a^{\dagger} (n+1) | n \rangle = (n+1) (a^{\dagger} | n \rangle) , \qquad (8.20)$$

and $a^{\dagger} | n \rangle$, if non-vanishing, is another eigenvector of N with eigenvalue n+1. It has raised the eigenvalue by one unit. It is customary to call a^{\dagger} creation or raising operator and a annihilation or lowering operator. Both are sometimes referred to as ladder operators. Let us compute the norm squared of $a | n \rangle$:

$$||a|n\rangle||^2 = \langle an|an\rangle = \langle n|a^{\dagger}a|n\rangle = \langle n|N|n\rangle = n\langle n|n\rangle. \tag{8.21}$$

Now $\langle n|n\rangle=1$ and if $a|n\rangle\neq 0$ then its norm squared must be strictly positive so that we conclude n>0. On the other hand we have $a|n\rangle=0$ iff n=0. Thus $n\geq 0$ and if n=0 is an eigenvalue, then $a|0\rangle=0$. We can now show that the eigenvalues of N are the non-negative integers. Suppose on the contrary that n is not a non-negative integer. Then there exists a positive integer k such that n-k is strictly between -1 and 0, and acting k times with a on $|n\rangle$ one gets an eigenvalue n'=n-k strictly between -1 and 0. But this contradicts the previously proven result that the eigenvalues must be $n'\geq 0$. The only way out of this contradiction is that n is a non-negative integer. Then applying n times the operator a one obtains the eigenvector with eigenvalue n'=0. Acting once more with a then results in $a|n'=0\rangle=0$ so that the series stops and no negative eigenvalue (and corresponding state with negative norm squared) is generated. Then, starting from this eigenstate $|0\rangle$ with lowest eigenvalue n=0 we can generate all positive integer eigenvalues and eigenvectors by acting with a^{\dagger} multiple times. Indeed, we have shown in (8.20) that $a^{\dagger}|n\rangle$, if non-vanishing, is eigenvector of N with eigenvector n+1. But the norm squared of this state is $||a^{\dagger}|n\rangle||^2 = \langle n|aa^{\dagger}|n\rangle = \langle n|(N+1)|n\rangle = (n+1) > 0$, so $a^{\dagger}|n\rangle$ is never vanishing. Moreover, the correctly normalised states are

$$|n+1\rangle = \frac{1}{\sqrt{n+1}} a^{\dagger} |n\rangle \quad , \quad |n-1\rangle = \frac{1}{\sqrt{n}} a |n\rangle \quad , \quad a |0\rangle = 0 .$$
 (8.22)

We may rewrite this equivalently as

$$a^{\dagger} |n\rangle = \sqrt{n+1} |n+1\rangle$$
 , $a|n\rangle = \sqrt{n} |n-1\rangle$, $a|0\rangle = 0$. (8.23)

Iterating, one finds

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^{\dagger})^n |0\rangle . \tag{8.24}$$

Coming back to the Hamiltonian, we immediately see that

$$H|n\rangle = E_n|n\rangle$$
 , $E_n = \hbar\omega(n + \frac{1}{2})$, $n = 0, 1, 2, ...$ (8.25)

In particular, the ground state energy is $E_0 = \frac{\hbar\omega}{2}$.

8.2 Expectation values of X^n and P^n

It is now relatively easy to compute expectation values of various powers of X and P. First of all,

$$\langle n' | (a^{\dagger})^k | n \rangle = \sqrt{(n+1)(n+2) \times \dots (n+k)} \langle n' | n+k \rangle = \sqrt{(n+1)(n+2) \times \dots (n+k)} \, \delta_{n',n+k} ,$$

 $\langle n' | a^k | n \rangle = \sqrt{n(n-1) \times \dots (n-k+1)} \, \delta_{n',n-k} .$ (8.26)

In particular, for n' = n all these vanish except for k = 0. It then follows from the expressions (8.6) of X and P that

$$\langle n|X|n\rangle = \langle n|P|n\rangle = 0$$
. (8.27)

Similarly, looking at the expressions of X^2 and P^2 given in (8.11) and (8.12) we see that in $\langle n|X^2|n\rangle$ or in $\langle n|P^2|n\rangle$ the terms $\sim aa$ or $\sim a^{\dagger}a^{\dagger}$ cannot contribute, while the $a^{\dagger}a=N$ just gives n so that

$$\frac{m}{2}\omega^{2}\langle n|X^{2}|n\rangle = \frac{\hbar\omega}{4}(2n+1) = \frac{E_{n}}{2} \quad , \quad \frac{1}{2m}\langle n|P^{2}|n\rangle = \frac{\hbar\omega}{4}(2n+1) = \frac{E_{n}}{2} . \tag{8.28}$$

In particular, we see that the expectation value of the kinetic energy equals the expectation value of the potential energy. This is the quantum analogue of the classical Viriel theorem! We also see that

$$(\Delta X)_n^2 = \langle X^2 \rangle_n = \frac{\hbar}{2m\omega} (2n+1) \quad , \quad (\Delta P)_n^2 = \langle P^2 \rangle_n = \frac{\hbar m\omega}{2} (2n+1) \quad . \tag{8.29}$$

Then

$$\Delta X_n \, \Delta P_n = \hbar (n + \frac{1}{2}) \,\,, \tag{8.30}$$

and the minimal uncertainty is obtained for the ground state n=0 where one reaches the limit allowed by the Heisenberg uncertainty relation, namely $\Delta X \Delta P = \frac{\hbar}{2}$.

Just as for X and P, the expectation value of any odd power of X or of P vanishes in the eigenstate $|n\rangle$. This is because these odd powers always contain an odd number of a or a^{\dagger} and hence cannot contain any term with equal numbers of a and a^{\dagger} . However, the even powers have non-vanishing expectation values. Let us then compute $\langle n|X^4|n\rangle$. If we expand $(a+a^{\dagger})^4$ we only need to retain the terms with two a and two a^{\dagger} . There are $\binom{4}{2}=6$ such terms, but they occur in all possible orders. Instead we will proceed slightly differently:

$$\langle n | (a + a^{\dagger})^{4} | n \rangle = \sum_{k \geq 0} \langle n | (a + a^{\dagger})^{2} | k \rangle \langle k | (a + a^{\dagger})^{2} | n \rangle = \sum_{k \geq 0} |\langle k | (a + a^{\dagger})^{2} | n \rangle|^{2}$$

$$= \sum_{k = n - 2, n, n + 2} |\langle k | (aa + a^{\dagger}a^{\dagger} + 2a^{\dagger}a + 1) | n \rangle|^{2}$$

$$= |\langle n - 2 | aa | n \rangle|^{2} + |\langle n + 2 | a^{\dagger}a^{\dagger} | n \rangle|^{2} + |\langle n | (aa^{\dagger} + a^{\dagger}a) | n \rangle|^{2}$$

$$= n(n - 1) + (n + 1)(n + 2) + (2n + 1)^{2} = 3(2n^{2} + 2n + 1) . \tag{8.31}$$

Similarly also

$$\langle n | (a - a^{\dagger})^4 | n \rangle = 3(2n^2 + 2n + 1) .$$
 (8.32)

It may look surprising that one gets the same result, but the extra minus sign only affects the terms in the expansion of $(a-a^{\dagger})^4$ that involve odd powers of a^{\dagger} and these terms do not contribute. Then

$$\langle n | X^4 | n \rangle = \frac{3\hbar^2}{4m^2\omega^2} (2n^2 + 2n + 1) \quad , \quad \langle n | P^4 | n \rangle = \frac{3\hbar^2 m^2\omega^2}{4} (2n^2 + 2n + 1) .$$
 (8.33)

In the beginning of this section we remarked that for the harmonic oscillator the mean values of position and energy should satisfy the classical equations of motion due to Ehrenfest's theorem and the fact that V'(X) is linear in X. This means they should oscillate with angular frequency ω . We have just seen that for an eigenstate of the Hamiltonian $\langle X \rangle_n = \langle P \rangle_n = 0$. This certainly is a solution of the classical equations of motion, but a trivial one. To see some time-dependence we need (as always) to look at some superposition of eigenstates. Solving the Schrödinger equation gives the general solution

$$|\psi(t)\rangle = \sum_{n\geq 0} e^{-iE_n t/\hbar} c_n(0) |n\rangle \quad , \quad \sum_{n\geq 0} |c_n(0)|^2 = 1 .$$
 (8.34)

Then, using (8.26), we have

$$\langle X \rangle_{\psi(t)} = \langle \psi(t) | X | \psi(t) \rangle = \sum_{n,k \geq 0} e^{-i(E_n - E_k)t/\hbar} c_k^*(0) c_n(0) \langle k | X | n \rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \sum_{n,k \geq 0} e^{-i(E_n - E_k)t/\hbar} c_k^*(0) c_n(0) \left(\sqrt{n+1}\delta_{k,n+1} + \sqrt{n}\delta_{k,n-1}\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left(\sum_{n \geq 0} e^{i\omega t} c_{n+1}^*(0) c_n(0) \sqrt{n+1} + \sum_{k \geq 0} e^{-i\omega t} c_k^*(0) c_{k+1}(0) \sqrt{k+1}\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \left(\sum_{n \geq 0} e^{i\omega t} c_{n+1}^*(0) c_n(0) \sqrt{n+1} + \text{c.c.}\right), \tag{8.35}$$

(where +c.c. means to add the complex conjugate expression). Similarly,

$$\langle P \rangle_{\psi(t)} = \langle \psi(t) | P | \psi(t) \rangle = \sum_{n,k \geq 0} e^{-i(E_n - E_k)t/\hbar} c_k^*(0) c_n(0) \langle k | P | n \rangle$$

$$= i \sqrt{\frac{\hbar m \omega}{2}} \sum_{n,k \geq 0} e^{-i(E_n - E_k)t/\hbar} c_k^*(0) c_n(0) \left(\sqrt{n+1} \delta_{k,n+1} - \sqrt{n} \delta_{k,n-1}\right)$$

$$= i \sqrt{\frac{\hbar m \omega}{2}} \left(\sum_{n \geq 0} e^{i\omega t} c_{n+1}^*(0) c_n(0) \sqrt{n+1} - \sum_{k \geq 0} e^{-i\omega t} c_k^*(0) c_{k+1}(0) \sqrt{k+1}\right)$$

$$= i \sqrt{\frac{\hbar m \omega}{2}} \left(\sum_{n \geq 0} e^{i\omega t} c_{n+1}^*(0) c_n(0) \sqrt{n+1} - \text{c.c.}\right). \tag{8.36}$$

Note that both $\langle X \rangle_{\psi(t)}$ and $\langle P \rangle_{\psi(t)}$ are real, as they should. Moreover, we now explicitly see that the various terms oscillate with a frequency ω and that

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle_{\psi(t)} = \frac{\langle P\rangle_{\psi(t)}}{m} \quad , \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle_{\psi(t)} = -m\omega^2\langle X\rangle_{\psi(t)} . \tag{8.37}$$

While the time evolutions of these mean values behave like the classical x and p, they no longer correspond to minimum uncertainty since we have seen that for an energy eigenstate the minimum uncertainty is only obtained for the ground state. Here we superpose at least two states, and one

can check that $(\Delta X)_{\psi(t)}(\Delta P)_{\psi(t)} > \frac{\hbar}{2}$. In the next subsection, we will construct states that mimic the classical physics as closely as possible, by (i) having minimal uncertainty and (ii) such that $\langle X \rangle$ and $\langle P \rangle$ satisfy the classical equations of motion. These are the so-called coherent states.

8.3 Coherent states

We could obtain the coherent states from these two requirements. But let us proceed differently and then check that these two conditions are satisfied. So here we define the coherent state $|\alpha\rangle$ as the eigenstate of the non-hermitian lowering operator a:

$$a |\alpha\rangle = \alpha |\alpha\rangle \quad , \quad \alpha \in \mathbf{C} .$$
 (8.38)

Since a is not hermitian, there is no reason for the eigenvalue to be real. Let us write $|\alpha\rangle = \sum_{n\geq 0} c_n |n\rangle$. Then the previous equation is $\sum_{n\geq 1} c_n \sqrt{n} |n-1\rangle = \alpha \sum_{n\geq 0} c_n |n\rangle$. Shifting the index in the sum on the left-hand side one sees that $\sqrt{n+1} c_{n+1} = \alpha c_n$ so that $c_n = \frac{\alpha}{\sqrt{n}} c_{n-1}$ which leads to $c_n = \frac{\alpha^n}{\sqrt{n!}} c_0$, or using further (8.24), $|\alpha\rangle = c_0 \sum_{n\geq 0} \frac{\alpha^n (a^{\dagger})^n}{n!} |0\rangle$. To summarise:

$$|\alpha\rangle = c_0 e^{\alpha a^{\dagger}} |0\rangle , \qquad (8.39)$$

where the constant c_0 is to be determined by the normalisation:

$$1 = \langle \alpha | \alpha \rangle = |c_0|^2 \langle 0| e^{\alpha^* a} e^{\alpha a^{\dagger}} | 0 \rangle . \tag{8.40}$$

To evaluate this, it is helpful to first prove the following two very useful formula:

Exercise 8.1: Let A and B be two linear operators. Show that

$$e^{A}Be^{-A} = B + [A, B] + \frac{1}{2}[A, [A, B]] + \frac{1}{6}[A, [A, A, B]] + \dots$$
 (8.41)

Exercise 8.2: Baker-Campbell-Haussdorf formula: Similarly show that

$$e^{A}e^{B} = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A,[A,B]]+\frac{1}{12}[B,[B,A]]+\dots}$$
(8.42)

where the unwritten terms $+ \dots$ involve triple (and higher) commutators. In particular if [A, B] commutes with A and with B one simply has the Glauber formula

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]} \Leftrightarrow e^A e^B = e^{\frac{1}{2}[A,B]} e^{A+B}$$
, if $[A, [A, B]] = [B, [A, B]] = 0$. (8.43)

Applying this formula twice one also has

$$e^A e^B = e^{[A,B]} e^B e^A$$
, if $[A, [A, B]] = [B, [A, B]] = 0.$ (8.44)

Choosing $A = \alpha^* a$ and $B = \alpha a^{\dagger}$ gives

$$e^{\alpha^* a} e^{\alpha a^{\dagger}} = e^{|\alpha|^2} e^{\alpha a^{\dagger}} e^{\alpha^* a} , \qquad (8.45)$$

so that

$$\langle 0| e^{\alpha^* a} e^{\alpha a^{\dagger}} |0\rangle = e^{|\alpha|^2} \langle 0| e^{\alpha a^{\dagger}} e^{\alpha^* a} |0\rangle = e^{|\alpha|^2}. \tag{8.46}$$

since $e^{\alpha^* a} |0\rangle = \sum_k \frac{(\alpha^*)^k}{n!} a^k |0\rangle = |0\rangle$. Finally then, for the normalisation we get $c_0 = e^{-|\alpha|^2/2}$, and

$$\left| |\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^{\dagger}} |0\rangle = e^{-|\alpha|^2/2} \sum_{n\geq 0} \frac{\alpha^n}{\sqrt{n!}} |n\rangle . \right|$$
 (8.47)

We can again apply the Glauber formula (8.43) to rewrite this in a still different form. We take $A = \alpha a^{\dagger}$ and $B = -\alpha^* a$ to get $e^{\alpha a^{\dagger}} e^{-\alpha^* a} = e^{|\alpha|^2/2} e^{\alpha a^{\dagger} - \alpha^* a}$, and applying this to $|0\rangle$ we see that we get another writing of the coherent state $|\alpha\rangle$ as

$$|\alpha\rangle = e^{\alpha a^{\dagger} - \alpha^* a} |0\rangle . \tag{8.48}$$

On the other hand, $-ibP/\hbar = -i\frac{b}{\sqrt{2}\gamma}\frac{a-a^{\dagger}}{i} = \frac{b}{\sqrt{2}\gamma}(a^{\dagger}-a)$ and identifying $\alpha = \frac{b}{\sqrt{2}\gamma}$ we see that for real α we have

$$|\alpha\rangle = e^{-i\sqrt{2}\gamma\alpha P/\hbar}|0\rangle$$
 , for real α . (8.49)

But $e^{-i\sqrt{2}\gamma\alpha P/\hbar} = T(\sqrt{2}\gamma\alpha)$ is the translation operator (cf. (6.52)) that acts as $\langle x|T(\sqrt{2}\gamma\alpha) = \langle x-\sqrt{2}\gamma\alpha|$. Hence for real α , the coherent state is a displaced ground state.³⁹ We will see this again below when we apply a uniform electric field to a charged particle in the harmonic potential.

From the second writing in (8.47) we can immediately deduce the time evolution by multiplying each $|n\rangle$ by $e^{-iE_nt/\hbar} = e^{-i\omega t/2 - in\omega t}$. This results in an overall factor $e^{-i\omega t/2}$ and the replacement of α by $\alpha e^{-i\omega t}$:

$$|\alpha, t\rangle = e^{-i\omega t/2} |e^{-i\omega t}\alpha\rangle = e^{-i\omega t/2} e^{-|\alpha|^2/2} e^{\alpha e^{-i\omega t}a^{\dagger}} |0\rangle . \tag{8.50}$$

We see that the coherent state remains a coherent state with the same $|\alpha|$ but time-varying phase. In particular, even if we start with a real α this will not remain real.

We now want to show that these coherent states $|\alpha\rangle$ form a "basis", although an over-complete and non-orthonormal one. First, one finds for the inner product of two coherent states

$$\langle \beta \, | \alpha \rangle = e^{-\frac{1}{2}(|\alpha|^2 + |\beta|^2)} \, \langle 0 | \, e^{\beta^* a} e^{\alpha a^\dagger} \, | 0 \rangle = e^{-\frac{1}{2}(|\alpha|^2 + |\beta|^2) + \beta^* \alpha} \quad \Rightarrow \quad |\langle \beta \, | \alpha \rangle \, |^2 = e^{-|\alpha - \beta|^2} \, \, . \tag{8.51}$$

Next we want to show the analogue of the completeness relation by summing $|\alpha\rangle\langle\alpha|$ over all α . Now, since α is complex, one should integrate over the real and imaginary part of α . We will set $\alpha = \alpha_x + i\alpha_y = r\,e^{i\phi}$ so that $\mathrm{d}^2\alpha = r\mathrm{d}r\mathrm{d}\phi$. Then, using $\int_0^{2\pi}\mathrm{d}\phi\,e^{i(n-m)\phi} = 2\pi\delta_{nm}$ we have

$$\frac{1}{\pi} \int d^2 \alpha |\alpha\rangle \langle \alpha| = \frac{1}{\pi} \int d^2 \alpha e^{-|\alpha|^2} \sum_{n,m \geq 0} \frac{\alpha^n}{\sqrt{n!}} \frac{(\alpha^*)^m}{\sqrt{m!}} |n\rangle \langle m|$$

$$= \frac{1}{\pi} \int_0^\infty dr \, r \int_0^{2\pi} d\phi \, e^{-r^2} \sum_{n,m \geq 0} \frac{r^n e^{in\phi}}{\sqrt{n!}} \frac{r^m e^{-im\phi}}{\sqrt{m!}} |n\rangle \langle m| = 2 \int_0^\infty dr \, r \, e^{-r^2} \sum_{n \geq 0} \frac{r^{2n}}{n!} |n\rangle \langle n| . \quad (8.52)$$

³⁹Of course, this "displaced ground state" is *not* the ground state of the Hamiltonian (8.2) but of a different Hamiltonian that would have another harmonic potential with a minimum at $\sqrt{2}\gamma\alpha$.

But $2\int_0^\infty dr \, r \, e^{-r^2} r^{2n} = \int_0^\infty d\xi e^{-\xi} \xi^n = n!$, so that

$$\frac{1}{\pi} \int d^2 \alpha |\alpha\rangle \langle \alpha| = \sum_{n \ge 0} |n\rangle \langle n| = \mathbf{1} . \tag{8.53}$$

We finally compute the mean energy, position, momentum and their uncertainties. First, using $N = a^{\dagger}a$ and $a |\alpha\rangle = \alpha |\alpha\rangle$ as well as the hermitian conjugate equation $\langle \alpha | a^{\dagger} = \langle \alpha | \alpha^* \rangle$ we get

$$\langle N \rangle_{\alpha} = \langle \alpha | a^{\dagger} a | \alpha \rangle = |\alpha|^2$$
 (8.54)

so that

$$\langle H \rangle_{\alpha} = \langle \alpha | H | \alpha \rangle = \hbar \omega \left(|\alpha|^2 + \frac{1}{2} \right) .$$
 (8.55)

Next,

$$\langle X \rangle_{\alpha} = \sqrt{\frac{\hbar}{2m\omega}} \langle \alpha | (a + a^{\dagger}) | \alpha \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\alpha + \alpha^{*}) ,$$

$$\langle X^{2} \rangle_{\alpha} = \frac{\hbar}{2m\omega} \langle \alpha | (aa + a^{\dagger}a^{\dagger} + 2a^{\dagger}a + 1) | \alpha \rangle = \frac{\hbar}{2m\omega} (\alpha^{2} + \alpha^{*2} + 2\alpha^{*}\alpha + 1)$$

$$= \langle X \rangle_{\alpha}^{2} + \frac{\hbar}{2m\omega} ,$$
(8.56)

as well as

$$\langle P \rangle_{\alpha} = \sqrt{\frac{\hbar m \omega}{2}} i \langle \alpha | (a^{\dagger} - a) | \alpha \rangle = \sqrt{\frac{\hbar m \omega}{2}} i (a^* - a) ,$$

$$\langle P^2 \rangle_{\alpha} = \frac{\hbar m \omega}{2} \langle \alpha | (-aa - a^{\dagger}a^{\dagger} + 2a^{\dagger}a + 1) | \alpha \rangle = \frac{\hbar m \omega}{2} (-\alpha^2 - \alpha^{*2} + 2\alpha^*\alpha + 1)$$

$$= \langle P \rangle_{\alpha}^2 + \frac{\hbar m \omega}{2} . \tag{8.57}$$

It follows that

$$(\Delta X)_{\alpha}^{2} = \frac{\hbar}{2m\omega} \quad , \quad (\Delta P)_{\alpha}^{2} = \frac{\hbar m\omega}{2} \quad \Rightarrow \quad \Delta X_{\alpha} \Delta P_{\alpha} = \frac{\hbar}{2} .$$
 (8.58)

Hence the coherent states are minimal uncertainly states, and since a coherent state remains coherent under time evolution, it remains a minimal uncertainty state over time. We obviously have (with $\alpha = |\alpha|e^{i\delta}$)

$$\langle X \rangle_{\alpha(t)} = \sqrt{\frac{\hbar}{2m\omega}} \left(\alpha e^{-i\omega t} + \alpha^* e^{i\omega t} \right) = \sqrt{\frac{2\hbar}{m\omega}} |\alpha| \cos(\omega t - \delta) ,$$

$$\langle P \rangle_{\alpha(t)} = \sqrt{\frac{\hbar m\omega}{2}} i \left(\alpha^* e^{i\omega t} - \alpha e^{-i\omega t} \right) = -\sqrt{2\hbar m\omega} |\alpha| \sin(\omega t - \delta) , \qquad (8.59)$$

and one again easily verifies that these expectation values satisfy the classical equations of motion of the harmonic oscillator :

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle_{\alpha(t)} = \frac{1}{m}\langle P\rangle_{\alpha(t)} \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle_{\alpha(t)} = -m\omega^2\langle X\rangle_{\alpha(t)} \ . \tag{8.60}$$

8.4 Hermite polynomials

We will now explicitly work out the eigenfunctions $\varphi_n(x) = \langle x | n \rangle$. While there is not really any need to do so - we can obtain almost any desired information working in the algebraic approach used so far - it is nevertheless nice to see at least one explicit example of an orthonormal basis in $L^2(\mathbf{R})$.

We begin with the ground state wave function $\varphi_0(x) = \langle x | 0 \rangle$. We exploit the characterisation of the ground state as $a | 0 \rangle = 0$ and write

$$0 = \langle x | a | 0 \rangle = \frac{1}{\sqrt{2}} \langle x | \left(\sqrt{\frac{m\omega}{\hbar}} X + \frac{i}{\sqrt{m\omega\hbar}} P \right) | 0 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\frac{\mathrm{d}}{\mathrm{d}x} + \frac{m\omega}{\hbar} x \right) \varphi_0(x) . \tag{8.61}$$

This constitutes a first order differential equation for φ_0 with solution

$$\varphi_0(x) = Ae^{-\frac{m\omega}{2\hbar}x^2} , \qquad (8.62)$$

where A is a (conventionally real and positive) normalisation constant which is determined by

$$1 = \int_{-\infty}^{\infty} dx \, |\varphi_0(x)|^2 = |A|^2 \int_{-\infty}^{\infty} dx \, e^{-\frac{m\omega}{\hbar}x^2} = |A|^2 \sqrt{\frac{\hbar\pi}{m\omega}} \quad \Rightarrow \quad A = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \,, \tag{8.63}$$

so that

$$\varphi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} . \tag{8.64}$$

Recall that in (8.4) we had introduced the characteristic length scale $\gamma = \sqrt{\frac{\hbar}{m\omega}}$ in terms of which we can rewrite this as $\varphi_0(x) = (\gamma \pi)^{-1/4} e^{-x^2/(2\gamma^2)}$. It is then useful to introduce the rescaled coordinate $\hat{x} = \frac{x}{\gamma}$, in terms of which $\varphi_0(x) = (\gamma \pi)^{-1/4} e^{-\hat{x}^2/2}$. The definition (8.5) of a^{\dagger} and the relation (8.23) then become

$$\sqrt{n}\varphi_n(x) = \sqrt{n}\langle x | \varphi_n \rangle = \langle x | a^{\dagger} | \varphi_{n-1} \rangle = \frac{1}{\sqrt{2}} \left(\frac{x}{\gamma} - \gamma \frac{\mathrm{d}}{\mathrm{d}x} \right) \langle x | \varphi_{n-1} \rangle = \frac{1}{\sqrt{2}} \left(\hat{x} - \frac{\mathrm{d}}{\mathrm{d}\hat{x}} \right) \langle x | \varphi_{n-1} \rangle
= \frac{1}{\sqrt{2}} \left(\hat{x} - \frac{\mathrm{d}}{\mathrm{d}\hat{x}} \right) \varphi_{n-1}(x) .$$
(8.65)

Iterating this relation n times we get

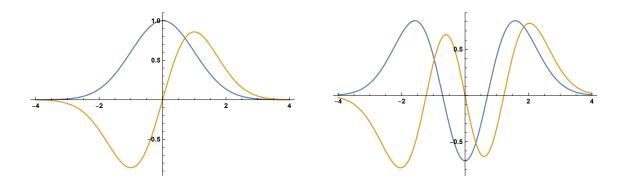
$$\varphi_n(x) = (\gamma \pi)^{-1/4} \frac{1}{\sqrt{2^n n!}} (\hat{x} - \frac{\mathrm{d}}{\mathrm{d}\hat{x}})^n e^{-\hat{x}^2/2} \quad , \qquad \hat{x} = \frac{x}{\gamma} = \sqrt{\frac{m\omega}{\hbar}} x .$$
(8.66)

It is easy to see that acting n times with $\hat{x} - \frac{d}{d\hat{x}}$ on $e^{-\hat{x}^2/2}$ gives $e^{-\hat{x}^2/2}$ times a polynomial of degree n. By definition, the resulting polynomial is the nth Hermite polynomial H_n . More precisely,

$$\varphi_n(x) = (\gamma \pi)^{-1/4} \frac{1}{\sqrt{2^n n!}} e^{-\hat{x}^2/2} H_n(\hat{x}) \quad , \quad H_n(\hat{x}) = e^{\hat{x}^2/2} (\hat{x} - \frac{\mathrm{d}}{\mathrm{d}\hat{x}})^n e^{-\hat{x}^2/2} . \tag{8.67}$$

Explicitly we have

$$H_0(\hat{x}) = 1$$
, $H_1(\hat{x}) = 2\hat{x}$, $H_2(\hat{x}) = 4\hat{x}^2 - 2$, $H_3(\hat{x}) = 8\hat{x}^3 - 12\hat{x}$. (8.68)



The figures shows the first few harmonic oscillator wave functions, φ_0 (blue) and φ_1 (yellow) on the left figure and φ_2 (blue) and φ_3 (yellow) on the right figure.

While we defined the Hermite polynomials by (8.67), one often encounters another definition:

$$H_n(\hat{x}) = (-)^n e^{\hat{x}^2} \frac{\mathrm{d}^n}{\mathrm{d}\hat{x}^n} e^{-\hat{x}^2} . \tag{8.69}$$

It is easy to compute the first few H_n from this formula and check that they coincide with the explicit H_n given in (8.68) as computed from (8.67). The general proof is also easy:

Exercise 8.3: Show that

$$\frac{\mathrm{d}}{\mathrm{d}\hat{x}} \left(e^{-\hat{x}^2/2} f(\hat{x}) \right) = e^{-\hat{x}^2/2} \left(\frac{\mathrm{d}}{\mathrm{d}\hat{x}} - \hat{x} \right) f(\hat{x}) . \tag{8.70}$$

Deduce the corresponding formula for $\left(\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\right)^n \left(e^{-\hat{x}^2/2}f(\hat{x})\right)$. By setting $f(\hat{x}) = e^{-\hat{x}^2/2}$, one then obtains the equality of the two expressions for H_n .

8.5 Harmonic oscillator at finite temperature : canonical ensemble

Suppose we have a large number N of identical harmonic oscillators. This could be e.g. a gas of diatomic molecules. In this case their number is of the order of Avogadro's number $N_A \simeq 10^{23}$. At finite temperature T, statistical physics tells us that the probability p_n that a given oscillator has energy E_n is given by the Boltzmann distribution as

$$p_n = \frac{1}{Z}e^{-E_n/(k_BT)} = \frac{1}{Z}e^{-\beta E_n} = \frac{1}{Z}e^{-\beta\hbar\omega(n+\frac{1}{2})}$$
, $\beta = \frac{1}{k_BT}$, (8.71)

and where the so-called partition function Z serves to normalise the probabilities $(\sum_n p_n = 1)$ which implies

$$Z = \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_{n=0}^{\infty} e^{-\beta \hbar \omega (n + \frac{1}{2})} = \frac{e^{-\beta \hbar \omega / 2}}{1 - e^{-\beta \hbar \omega}} = \left(2 \sinh \beta \hbar \omega / 2\right)^{-1}$$
(8.72)

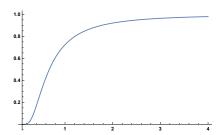
This can be rephrased by saying that the density matrix is

$$\rho = \sum_{n=0}^{\infty} p_n |n\rangle \langle n| = \frac{1}{Z} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})} |n\rangle \langle n| . \qquad (8.73)$$

We can then compute the statistical average of the quantum mean energies (the mean energy per oscillator U/N) as

$$\frac{U}{N} \equiv \langle \langle H \rangle \rangle = \operatorname{tr} \rho H = \sum_{n=0}^{\infty} p_n E_n = \frac{1}{Z} \sum_{n=0}^{\infty} e^{-\beta E_n} E_n = -\frac{\partial}{\partial \beta} \log Z = \frac{\hbar \omega}{2} \coth \frac{\beta \hbar \omega}{2} . \tag{8.74}$$

For small temperature (large β) one has $\coth \frac{\beta\hbar\omega}{2} \to 1$ and $U \simeq \frac{\hbar\omega}{2}N$ is independent of T. For large temperature (small β) one has $\coth \frac{\beta\hbar\omega}{2} \simeq \frac{2}{\beta\hbar\omega}$ and $U \simeq \frac{N}{\beta} = Nk_BT$. We see that at large temperature the specific heat (heat capacity) $C_V = \frac{\partial U}{\partial T}$ is constant and equals $Nk_B = \frac{N}{N_A}(N_Ak_B) = nR$ while at low temperature it goes to zero. More precisely, we have $\frac{\partial U}{\partial T} = \frac{\partial \beta}{\partial T} \frac{\partial U}{\partial \beta} = -\frac{1}{k_BT^2} \frac{\partial U}{\partial \beta} = Nk_B \frac{x^2}{\sinh^2 x}$ where $x = \frac{\hbar\omega}{2k_BT}$. In the figure we plotted $\frac{1}{Nk_B} \frac{\partial U}{\partial T} = \frac{x^2}{\sinh^2 x}$ as a function of $\frac{1}{x} = \frac{2k_BT}{\hbar\omega}$, and one sees again that the heat capacity goes to 0 at small temperature, while it goes to Nk_B at large temperatures (as soon as k_BT is larger than a few $\hbar\omega$).



8.6 Charged harmonic oscillator in a constant electric field

To close this section we look at an electrically charged particle in a (one-dimensional) harmonic potential and apply a constant and homogeneous electric field. The homogeneous electric field \mathcal{E} derives from an electrostatic potential $\Phi(x) = -\mathcal{E}x$ (in general $\vec{\mathcal{E}} = -\vec{\nabla}\Phi$) and hence adds a potential energy $q\Phi = -q\mathcal{E}x$. This should add a piece $-q\mathcal{E}X$ to the harmonic oscillator Hamiltonian (cf our discussion of the ammonia molecule in subsection 4.2). Classically, the potential is changed from $\frac{m}{2}\omega^2x^2$ to

$$V(x) = \frac{m}{2}\omega^2 x^2 - q\mathcal{E}x = \frac{m}{2}\omega^2 (x - x_0)^2 - \frac{m}{2}\omega^2 x_0^2 \quad , \quad x_0 = \frac{q\mathcal{E}}{m\omega^2} . \tag{8.75}$$

This does two things: it shifts the minimum of the potential from 0 to x_0 and adds some constant energy $-\frac{m}{2}\omega^2x_0^2$.

We will now recover the analogous results in the quantum mechanical setting. Since x_0 and $\gamma = \sqrt{\frac{\hbar}{m\omega}}$ now are two length scales it will be useful to trade x_0 , and hence \mathcal{E} , for γ and a dimensionless quantity $\eta = \frac{x_0}{\sqrt{2}\gamma}$ (similar to but different from the η introduced in subsection 4.2). Then

$$\eta = \frac{x_0}{\sqrt{2}\gamma} \quad \Rightarrow \quad q\mathcal{E}\gamma = m\omega^2 x_0 \gamma = \sqrt{2}\eta m\omega^2 \gamma^2 = \sqrt{2}\eta \hbar\omega ,$$
(8.76)

so that $q\mathcal{E}X = q\mathcal{E}\frac{\gamma}{\sqrt{2}}(a+a^{\dagger}) = \eta\hbar\omega(a+a^{\dagger})$. We then take as the Hamiltonian

$$H = \frac{P^2}{2m} + \frac{m}{2}\omega^2 X^2 - q\mathcal{E}X = \hbar\omega \left(a^{\dagger}a + \frac{1}{2} - \eta(a + a^{\dagger})\right). \tag{8.77}$$

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This suggests to define new operators

$$\widetilde{a} = a - \eta \quad \Leftrightarrow \quad \widetilde{a}^{\dagger} = a^{\dagger} - \eta \ . \tag{8.78}$$

(More generally for complex η one would have $\tilde{a}^{\dagger} = a^{\dagger} - \eta^*$). These shifted operators satisfy again

$$[\widetilde{a}, \widetilde{a}^{\dagger}] = \mathbf{1} , \qquad (8.79)$$

while the Hamiltonian now reads

$$H = \hbar\omega \left(\tilde{a}^{\dagger} \tilde{a} + \frac{1}{2} - \eta^2 \right) . \tag{8.80}$$

We can then immediately conclude that the eigenvalues are

$$E_n = \hbar\omega \left(n + \frac{1}{2} - \eta^2\right) = \hbar\omega \left(n + \frac{1}{2}\right) - \frac{m}{2}\omega^2 x_0^2.$$
 (8.81)

The eigenvectors now are

$$|\widetilde{n}\rangle = \frac{(\widetilde{a}^{\dagger})^n}{\sqrt{n!}}|\widetilde{0}\rangle \quad , \quad \widetilde{a}|\widetilde{0}\rangle = 0 \ .$$
 (8.82)

How are these states related to the basis states $|n\rangle$ for vanishing electric field? First, look at the ground state. $\tilde{a}|\tilde{0}\rangle = 0$ is equivalent to $a|\tilde{0}\rangle = \eta|\tilde{0}\rangle$. But this is the equation of a coherent state and we identify $|\tilde{0}\rangle$ with $|\eta\rangle$, and from (8.47) and (8.49)

$$|\widetilde{0}\rangle = |\eta\rangle = e^{-\eta^2/2} e^{\eta a^{\dagger}} |0\rangle = e^{-i\sqrt{2}\gamma\eta P/\hbar} |0\rangle .$$
 (8.83)

The last writing shows that the ground state in the presence of the electric field is the ground state $|0\rangle$ (without electric field), translated by $\sqrt{2}\gamma\eta=x_0$, as one might have expected. Of course, this translated ground state is a superposition of all original eigenstates $|n\rangle$. Similarly, one can show that the excited states in the presence of the electric field also are the translated excited states without electric field:

Exercise 8.4: Recall that $[a^{\dagger}, P] = i \frac{\hbar}{\sqrt{2}\gamma}$ and deduce

$$[a^{\dagger}, e^{-i\sqrt{2}\gamma\eta P/\hbar}] = \eta e^{-i\sqrt{2}\gamma\eta P/\hbar} \quad \Rightarrow \quad (a^{\dagger} - \eta)e^{-i\sqrt{2}\gamma\eta P/\hbar} = e^{-i\sqrt{2}\gamma\eta P/\hbar} a^{\dagger} . \tag{8.84}$$

Use this to show that

$$(\widetilde{a}^{\dagger})^{n}|\widetilde{0}\rangle = e^{-i\sqrt{2}\gamma\eta P/\hbar} (a^{\dagger})^{n} |0\rangle , \qquad (8.85)$$

and conclude that the $n^{\rm th}$ excited state in the presence of the electric field is just the translated $n^{\rm th}$ excited state without the electric field.

Classically we expect that this displacement induces a dipole moment. Let us check this quantum mechanically by computing the expectation value of the position operator X in the ground state $|\widetilde{0}\rangle$. Since this is $|0\rangle$ translated by $\sqrt{2}\gamma\eta$ we expect to find $\langle X\rangle_{\widetilde{0}} = \sqrt{2}\gamma\eta$. This is indeed what we get from using (8.56) with $\alpha = \alpha^* = \eta$:

$$\langle X \rangle_{\tilde{0}} = \sqrt{2}\gamma\eta \ . \tag{8.86}$$

This also means that there is an induced dipole moment $q(X)_{\widetilde{0}} = \frac{q^2 \mathcal{E}}{m\omega^2}$.

Exercise 8.5: Compute similarly the expectation value of X and the induced dipole moment in the n^{th} excited state $|\widetilde{n}\rangle = \frac{1}{\sqrt{n!}}(\widetilde{a}^{\dagger})^n|\widetilde{0}\rangle$. Hint: use (8.85) and (8.41).

8.7 Bogolyubov transformation

Finally, it is worth noting that (8.78) constitutes a very simple example of a Bogolyubov transformation. More generally, a Hamiltonian that is bilinear in the a and a^{\dagger} can be transformed to a harmonic oscillator Hamiltonian by the so-called Bogolyubov transformation. Start with a hermitian expression as

$$M = a^{\dagger} a + \epsilon a a + \epsilon^* a^{\dagger} a^{\dagger} + \eta a + \eta^* a^{\dagger} , \qquad (8.87)$$

with some complex numbers ϵ and η , constrained by $|\epsilon| < 1$. We define for some complex constants c and d to be determined ($|c|^2 < 1$)

$$b = \frac{1}{\sqrt{1 - |c|^2}} \left(a + c^* a^\dagger + d^* \right) \quad \Leftrightarrow \quad b^\dagger = \frac{1}{\sqrt{1 - |c|^2}} \left(a^\dagger + ca + d \right) \tag{8.88}$$

One verifies that

$$[b, b^{\dagger}] = \frac{1}{1 - |c|^2} \Big([a, a^{\dagger}] + |c|^2 [a^{\dagger}, a] \Big) = \mathbf{1} . \tag{8.89}$$

Exercise: Show that by an appropriate choice of c and d one can achieve

$$M = C^2 b^{\dagger} b + F \tag{8.90}$$

with
$$C^2 = \frac{(1-|c|^2)}{(1+|c|^2)}$$
 and $F = -\frac{|c|^2+|d|^2}{(1+|c|^2)}$.

It follows that the spectrum of M is $C^2(n+\frac{1}{2})+F$ with the eigenstates being $\frac{(b^{\dagger})^n}{\sqrt{n!}}|\widehat{0}\rangle$, where the new "ground state" $|\widehat{0}\rangle$ is determined by $b|\widehat{0}\rangle=0$. One can again write this out in terms of the a and a^{\dagger} , but it is clear again that this new ground state is a superposition of all "old" eigenstates $|n\rangle$.

Without going into any details, let us only mention that in relativistic quantum field theory one also deals with these creation and annihilation operators where they create particles from a vacuum (ground state) or annihilate them. There is actually an infinity of such operators $a_{\vec{p}}$ and $a_{\vec{p}}^{\dagger}$, one pair for every momentum mode of the relativistic particle. The vacuum (ground state) is defined by $a_{\vec{p}} |0\rangle = 0$. When doing quantum field theory in curved space-time one is led to do a Bogolyubov transformation and the appropriate vacuum for an observer in one region of space-time can be the vacuum of the $b_{\vec{p}}$, while for an observer in another region it is the vacuum of the $a_{\vec{p}}$. But when viewed from the other region the "b-vacuum" contains many a^{\dagger} -particles. It is along these lines that Hawking discovered the Hawking radiation as emitted by black holes. This radiation has all characteristics of thermal black body radiation (described by a density matrix corresponding to a statistical mixture), even if the initial black hole could have been (in principle) a pure quantum state. Now, under unitary time-evolution, a pure state remains a pure state and cannot evolve into a statistical mixture. This has fueled a heated debate for about the last half century about the validity or violation of unitary evolution in quantum mechanics.