

Harmonic Oscillator

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References:

Townsend = *A Modern Approach to Quantum Mechanics* by J. S. Townsend. Second edition (2012)

1 Notation

★ It is convenient to introduce dimensionless quantities when discussing the quantum harmonic oscillator. Here is the notation which will be used in these notes.

- Hamiltonian in terms of dimensioned quantities:

$$H = \frac{1}{2m}P^2 + \frac{1}{2}kX^2 = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2X^2 = \frac{1}{2}\left(-\frac{\hbar^2}{m}\frac{\partial^2}{\partial x^2} + m\omega^2X^2\right) \quad (1)$$

- The quantum oscillator has a

$$\text{characteristic length: } \xi = \sqrt{\hbar/m\omega} \quad (2)$$

$$\text{characteristic momentum: } \eta = \sqrt{\hbar m\omega} \quad (3)$$

$$\text{characteristic velocity: } \nu = \sqrt{\hbar\omega/m} \quad (4)$$

- Note dimensions: $\hbar \sim ml^2t^{-1}$ implies that $\xi \sim l$, $\eta \sim mlt^{-1}$, $\nu \sim lt^{-1}$.
- Note that $\xi\eta = \hbar$, $\nu = \eta/m$.

- Placing a bar over the symbol for an operator gives its dimensionless counterpart:

$$\bar{X} = X/\xi, \quad \bar{P} = P/\eta, \quad \bar{H} = H/\hbar\omega = \frac{1}{2}(\bar{P}^2 + \bar{X}^2). \quad (5)$$

- The commutator $[X, P] = i\hbar I$ becomes $[\bar{X}, \bar{P}] = iI$, with I the identity operator.

- Lowering (destruction) a and raising (creation) a^\dagger operators are defined as:

$$a = \frac{1}{\sqrt{2}}(\bar{X} + i\bar{P}), \quad a^\dagger = \frac{1}{\sqrt{2}}(\bar{X} - i\bar{P}). \quad (6)$$

- Note that since \bar{X} and \bar{P} are Hermitian, the definition of a^\dagger follows from that of a , and vice versa.

- In terms of a^\dagger and a :

$$\bar{X} = \frac{1}{\sqrt{2}}(a + a^\dagger), \quad \bar{P} = \frac{1}{i\sqrt{2}}(a - a^\dagger), \quad (7)$$

$$N = a^\dagger a, \quad \bar{H} = \frac{1}{2}(a^\dagger a + a a^\dagger) = a^\dagger a + \frac{1}{2} = N + \frac{1}{2}. \quad (8)$$

- Dimensionless position representation:

$$u := x/\xi, \quad \bar{X} = \text{multiplication by } u, \quad \bar{P} = -i\partial/\partial u, \quad (9)$$

$$a = \frac{1}{\sqrt{2}}\left(u + \frac{\partial}{\partial u}\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(u - \frac{\partial}{\partial u}\right), \quad \bar{H} = \frac{1}{2}\left(-\frac{\partial^2}{\partial u^2} + u^2\right). \quad (10)$$

- Dimensionless momentum representation:

$$v := p/\eta, \quad \bar{X} = i\partial/\partial v, \quad \bar{P} = \text{multiplication by } v, \quad (11)$$

$$a = \frac{i}{\sqrt{2}}\left(v + \frac{\partial}{\partial v}\right), \quad a^\dagger = \frac{-i}{\sqrt{2}}\left(v - \frac{\partial}{\partial v}\right), \quad \bar{H} = \frac{1}{2}\left(v^2 - \frac{\partial^2}{\partial v^2}\right). \quad (12)$$

2 Eigenstates of the Number Operator N

★ See the treatment in Townsend Sec. 7.3, which is also found in many other textbooks. The conclusion is that the eigenvalues of N must be nonnegative integers. Given some eigenket of N , others can be generated using raising and lowering operators. In particular there is a minimum eigenvalue of 0, and if $|0\rangle$ denotes the corresponding ket, one can generate an infinite collection of orthogonal kets:

$$|n\rangle = (1/\sqrt{n!})(a^\dagger)^n|0\rangle; \quad N|n\rangle = n|n\rangle; \quad \bar{H}|n\rangle = (n + \frac{1}{2})|n\rangle. \quad (13)$$

The factor of $1/\sqrt{n!}$ is needed for normalization, and the $+1$ phase in this definition of $|n\rangle$ is the standard convention.

3 Position and Momentum Representations of Number Eigenstates

★ See the treatment in Townsend Sec. 7.4. The ground state in the dimensionless position representation, $\phi_0(u) = \langle u|0\rangle$, is the solution to a differential equation, and when normalized (and using the conventional phase) it takes the form

$$\phi_0(u) = (\pi)^{-1/4} \exp[-u^2/2] \quad (14)$$

• Starting with $\phi_0(u)$ the other number eigenstates can be obtained by applying a^\dagger an appropriate number of times, see (13), where a^\dagger is the differential operator given in (10). The result is that

$$\langle u|n\rangle = \phi_n(u) \propto h_n(u) \exp[-u^2/2], \quad (15)$$

where $h_n(u)$ is the Hermite polynomial of degree n .

★ Number eigenstates in the dimensionless momentum representation can be obtained from those in the position representation, and vice versa, by means of a Fourier transform:

$$\langle v|n\rangle = \hat{\phi}_n(v) = \int_{-\infty}^{\infty} \langle v|u\rangle \langle u|n\rangle du = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-iuv} \phi_n(u) du; \quad (16)$$

$$\langle u|n\rangle = \phi_n(u) = \int_{-\infty}^{\infty} \langle u|v\rangle \langle v|n\rangle dv = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{iuv} \hat{\phi}_n(v) dv. \quad (17)$$

• It turns out that the wave functions for dimensionless momentum and position corresponding to $|n\rangle$ are identical apart from a phase:

$$\hat{\phi}_n(v) = (-i)^n \phi_n(u = v). \quad (18)$$

That is, start with the position space function $\phi_n(u)$, replace u everywhere with v , and multiply by $(-i)^n$ to obtain $\hat{\phi}_n(v)$.

◦ In particular, for $n = 0$,

$$\hat{\phi}_0(v) = (\pi)^{-1/4} \exp[-v^2/2] \quad (19)$$

□ Exercise. Assuming (16), prove the connection between $\hat{\phi}_n(v)$ and $\phi_n(u)$ stated in (18). [Hint: For $n = 0$ carry out the integral in (16). Then note that $\langle v|n\rangle$ can be obtained from $\langle v|0\rangle$ by repeated applications of a^\dagger in the momentum representation, see (12).]

4 Coherent States

4.1 Definition, properties, time dependence

★ Quantum states of a harmonic oscillator that actually oscillate in time cannot be energy eigenstates, which are stationary. The *coherent states* of a harmonic oscillator exhibit a temporal behavior which is similar to what one observes in a classical oscillator.

★ Definition. Let α be any complex number. Define

$$|\alpha\rangle := e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \quad (20)$$

◦ Coherent state kets $|\alpha\rangle$ should not be confused with number states $|n\rangle$. The nature of the argument (complex number vs. integer) can serve to distinguish them, or one can add an identifying subscript $|\alpha\rangle_c$ in cases where there might be confusion. In fact the states $|\alpha = 0\rangle$ and $|n = 0\rangle$ are identical, so at least they do not need to be distinguished.

□ Exercise. Show that the state defined in (20) is normalized: $\langle\alpha|\alpha\rangle = 1$.

★ The coherent state $|\alpha\rangle$ is an eigenket of the annihilation operator a with eigenvalue α ; likewise $\langle\alpha|$ is an eigenbra of the the creation operator with eigenvalue α^* :

$$a|\alpha\rangle = \alpha|\alpha\rangle; \quad \langle\alpha|a^\dagger = \alpha^*\langle\alpha| \quad (21)$$

□ Exercise. Verify $a|\alpha\rangle = \alpha|\alpha\rangle$ starting with the definition in (20).

• One can use (21) to find the matrix element of any product of powers of a and a^\dagger between two coherent states if they are in normal order: creation operators to the left of annihilation operators. Thus for p and q nonnegative integers,

$$\langle\alpha| (a^\dagger)^p a^q |\beta\rangle = (\alpha^*)^p \beta^q. \quad (22)$$

□ Exercise. Use (22) to show that

$$\langle\alpha|\bar{X}|\alpha\rangle = \sqrt{2} \operatorname{Re}(\alpha), \quad \langle\alpha|\bar{X}^2|\alpha\rangle = \frac{1}{2} + 2[\operatorname{Re}(\alpha)]^2. \quad (23)$$

□ Exercise. Evaluate $\langle\alpha|\bar{P}|\alpha\rangle$ and $\langle\alpha|\bar{P}^2|\alpha\rangle$.

★ The coherent states $|\alpha\rangle$ for different α are *not* orthogonal to each other, unlike the number states $|n\rangle$, or the states of the position representation, which are orthogonal in the formal sense of $\langle x|x'\rangle = \delta(x - x')$.

□ Exercise. Let α and β be two complex numbers. Find an expression for $\langle\alpha|\beta\rangle$. Show that its magnitude $|\langle\alpha|\beta\rangle|$ depends only on the absolute value $|\alpha - \beta|$ of the difference.

• Coherent states are *complete* in the sense that any $|\psi\rangle$ in the Hilbert space can be written, at least formally, as a sum or integral over a collection of coherent states. However, this can be done in more than one way, so one says that the set of coherent states is *over complete*.

• One can express the identity operator I as an integral of coherent-state dyads in various different ways. Here is one that is sometimes useful:

$$I = \frac{1}{\pi} \int_{-\infty}^{\infty} d\alpha' \int_{-\infty}^{\infty} d\alpha'' |\alpha'\rangle \langle\alpha''|, \quad (24)$$

where α' and α'' are the real and imaginary parts of α .

□ Exercise. Justify (24) by showing that it defines an operator with the property that $\langle n|I|n'\rangle = \delta_{nn'}$. Hint: Evaluate the double integral $\int d\alpha' \int d\alpha''$ in polar coordinates.

★ The time dependence of a coherent state can be worked out starting with

$$U(t)|n\rangle = e^{-i(n+1/2)\omega t}|n\rangle. \quad (25)$$

Thus

$$U(t)|\alpha\rangle = e^{-i\omega t/2} \sum_{n=0}^{\infty} \frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}} |n\rangle = e^{-i\omega t/2} |\alpha(t)\rangle \quad (26)$$

if we define

$$\alpha(t) := \alpha e^{-i\omega t}. \quad (27)$$

• That is to say, $\alpha(t)$ traces out a circle in the complex plane, moving clockwise as t increases. Just like the elliptical orbit of the point representing a classical oscillator in the x, p phase space, which of course can be made into a circle by choosing appropriate units for x and p .

□ Exercise. Let $\alpha(t) = r e^{-i\omega t}$, $r > 0$ a real number. Evaluate $\langle \alpha(t) | \bar{X} | \alpha(t) \rangle$ and $\langle \alpha(t) | \bar{P} | \alpha(t) \rangle$, and compare with what you would expect for a classical oscillator.

4.2 The displacement operator $D(\alpha)$

★ Define the *displacement operator* (the justification for this name will appear later)

$$D(\alpha) = \exp[\alpha a^\dagger - \alpha^* a], \quad (28)$$

where α is any complex number, and a and a^\dagger are the annihilation (lowering) and creation (raising) operators defined in Sec. 1.

• The operator $D(\alpha)$ is unitary, as follows from the observation that the exponent in (28) is anti-Hermitian or skew Hermitian, which means it is equal to its adjoint times a minus sign:

$$(\alpha a^\dagger - \alpha^* a)^\dagger = \alpha^* a - \alpha a^\dagger = -(\alpha a^\dagger - \alpha^* a). \quad (29)$$

Consequently,

$$D^\dagger(\alpha) = \exp[-\alpha a^\dagger + \alpha^* a] = [D(\alpha)]^{-1} = D(-\alpha). \quad (30)$$

★ The coherent state $|\alpha\rangle$ can be written as

$$|\alpha\rangle = D(\alpha)|0\rangle. \quad (31)$$

• To prove this it is helpful to have handy a formula for manipulating exponentials of two noncommuting operators A and B which have the property that their commutator $[A, B]$ commutes with *both* A and B :

$$[A, [A, B]] = 0 = [B, [A, B]]. \quad (32)$$

• Given this condition one can show (the argument is given in Townsend, p. 279, in the form of an exercise) that

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A, B]}. \quad (33)$$

• Let $A = \alpha a^\dagger$, $B = -\alpha^* a$. Then $[A, B] = |\alpha|^2 I$, which we will simply write as $|\alpha|^2$, and using (33) we see that $D(\alpha)$ in (28) can be rewritten as

$$D(\alpha) = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} e^{-\alpha^* a}. \quad (34)$$

We use this to evaluate

$$D(\alpha)|0\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} e^{-\alpha^* a}|0\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger}|0\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle, \quad (35)$$

where the right side coincides with the earlier definition of $|\alpha\rangle$ in (20).

◦ In writing (35) we have twice used the expansion $e^A = I + A + A^2/2! + \dots$. When $e^{-\alpha^*a}$ is expanded in this way and applied to $|0\rangle$ we get $|0\rangle$, for any positive power of a applied to $|0\rangle$ gives 0. The expansion of $e^{\alpha a^\dagger}$ applied to $|0\rangle$ gives the sum of the right side of (35) when one takes into account the $\sqrt{n!}$ that appears in (13).

□ Exercise. What is $D(\alpha)D(\beta)$ equal to? First make a guess (after all, if a displacement is followed by a second displacement, then...). Next show that your guess is correct up to a phase factor, which you should evaluate.

4.3 Wave packet in position space

★ As the next step we note that the exponent in the definition of $D(\alpha)$ can be written, using (6), in the form

$$\alpha a^\dagger - \alpha^* a = i\sqrt{2}[\alpha''\bar{X} - \alpha'\bar{P}], \text{ where } \alpha = \alpha' + i\alpha'' = \text{Re}(\alpha) + i\text{Im}(\alpha). \quad (36)$$

□ Exercise. Check it.

• As a consequence, setting $A = i\sqrt{2}\alpha''\bar{X}$ and $B = -i\sqrt{2}\alpha'\bar{P}$, and noting that $[\bar{X}, \bar{P}] = iI$, we can employ (33) to write

$$D(\alpha) = e^{-i\alpha'\alpha''} e^{i\sqrt{2}\alpha''\bar{X}} e^{-i\sqrt{2}\alpha'\bar{P}}. \quad (37)$$

★ We make use of (37) by noting that in the position representation, see (9), $\bar{P} = -i\partial/\partial u$, and hence

$$e^{-i\sqrt{2}\alpha'\bar{P}} = e^{-\sqrt{2}\alpha'(\partial/\partial u)} \quad (38)$$

is the operator which applied to some (nice) function $f(u)$ yields the shifted function $f(u - \sqrt{2}\alpha')$. As a consequence (37) allows us to write down an explicit form for $|\alpha\rangle$ in the position representation:

$$\phi(\alpha; u) := \langle u|\alpha\rangle = e^{-i\alpha'\alpha''} e^{i\sqrt{2}\alpha''u} \phi_0(u - \sqrt{2}\alpha'). \quad (39)$$

• It is helpful to explore the significance of (39) starting with the case in which $\alpha = \alpha' > 0$ is a positive real number. In that case, since $\alpha'' = 0$, (39) tells us that $\phi(\alpha; u)$ is simply the Gaussian function (14), the harmonic oscillator ground state, with its center shifted to the right by an amount $\sqrt{2}\alpha'$. Consequently, the mean of the corresponding probability distribution density for u , given by $|\phi(\alpha; u)|^2$ is $\sqrt{2}\alpha'$, and its standard deviation or “uncertainty” Δu is identical to that of the ground state.

◦ This justifies the name “displacement operator” for $D(\alpha)$, at least in the case in which α is real: it simply displaces the position-space wave function.

◦ But is it not an embarrassment, or at least an annoyance, that the displacement is $\sqrt{2}\alpha'$ and not α' ? Indeed, but there is not much one can do about it. One could employ a complex number $\bar{\alpha} = \sqrt{2}\alpha$ in place of α , but then there are factors of $\sqrt{2}$ in the exponent defining the displacement operator in terms of $\bar{\alpha}$. Or one could use a different definition for the characteristic length ξ of a harmonic oscillator. One way or another, a $\sqrt{2}$ will creep into the discussion.

• Returning to (39). What happens if α'' , the imaginary part of α is nonzero? First there is the phase factor $e^{-i\alpha'\alpha''}$, which has no effect on the physics represented by this state, so we will ignore it.

◦ If one is considering (which at the moment we are not) linear combinations of coherent states having different values of α , then one must pay some attention to these initial phases.

• The factor $e^{i\sqrt{2}\alpha''u}$, on the other hand, is a phase which depends upon the position u , so it has physical significance: it indicates that in addition to having a displaced position (assuming $\alpha' \neq 0$) the wave packet also has some momentum associated with it; that is, it represents a particle which is moving.

◦ In particular, the probability distribution for momentum, given by a symmetrical Gaussian distribution when $\alpha'' = 0$, is shifted in the dimensionless momentum variable v by an amount $\sqrt{2}\alpha''$.

□ Exercise. Work out the corresponding description of a wave packet in momentum space using the analog of (37), but with the \bar{P} and \bar{X} exponentials in the opposite order.

★ As a function of time α moves clockwise on a circle in the complex plane. Let us suppose that

$$\sqrt{2}\alpha = \sqrt{2}\alpha' + i\sqrt{2}\alpha'' = b(\cos \tau - i \sin \tau), \text{ where } \tau := \omega t \quad (40)$$

is the dimensionless time.

- Then aside from an overall phase, the position-space wave packet is

$$\phi(u, \tau) = e^{i(-b \sin \tau)u} \phi_0(u - b \cos \tau), \quad (41)$$

where remember that $\phi_0(u)$, (14), is a Gaussian centered at $u = 0$.

- The explicit function given in (41) provides a nice way of visualizing what happens as (dimensionless) time τ increases. The probability distribution density for position,

$$\rho(u, \tau) = |\phi(u, \tau)|^2 = [\phi_0(u - b \cos \tau)]^2, \quad (42)$$

is that of the ground state shifted by a distance $b \cos \tau$. So one can think of the wave packet as oscillating back and forth while maintaining its Gaussian shape.

- In addition there is a position-dependent phase $e^{i(-b \sin \tau)u}$ which tells us that the (dimensionless) momentum v has an average value of $-b \sin \tau$ corresponding to a nonzero average velocity. This is zero when τ is a multiple of π , i.e., when the (average) position u reaches its maximum or minimum value. Similarly, when τ is $\pi/2$ plus an integer times π , the (average) position is zero, and the momentum or velocity reaches its maximum or minimum value. This corresponds quite well with the motion of a classical oscillator.

- Of course, neither position nor momentum is precisely defined in a coherent state, and in dimensionless units the associated uncertainties are of the order of 1. Taking this into account one can visualize the wave packet, roughly speaking, as a circular orbit in the classical phase space, but “smudged out” a bit in both position and momentum.

◦ In the case in which $b \gg 1$ this “smudging out” is a relatively minor effect in comparison with the overall motion, and the classical picture becomes a quite good approximation to the behavior of the quantum oscillator in a coherent state.

- The nice correspondence between quantum unitary time development and a classical orbit is special to the harmonic oscillator. For other potentials, for example a square well or a Coulomb potential, unitary time development is not well approximated by a classical orbit, and the Ehrenfest relations, while they remain formally correct, can be quite misleading.

- ★ The probability current in dimensionless form corresponding to (41) is given by

$$j = \text{Im}(\phi^* \partial \phi / \partial u) = -(b \sin \tau) [\phi_0(u - b \cos \tau)]^2. \quad (43)$$

- Thus for a coherent state (but not for a general harmonic oscillator state) the probability current at a particular time is proportional to the probability distribution density (42). This reflects the fact that the latter moves “rigidly” as time progresses, i.e., without changing its shape.

- Exercise. Check that the (dimensionless) probability conservation equation

$$\partial \rho / \partial t = -\partial j / \partial x \quad (44)$$

is satisfied when ρ is given by (42) and j by (43).