

This means that, if we find an observable \hat{A} that commute with the Hamiltonian ($[\hat{A}, \hat{H}] = 0$), then we can simplify the eigenvalue equation $\hat{H}|\psi_E\rangle = E|\psi_E\rangle$, by looking for the eigenvectors of \hat{H} in each eigenspace of \hat{A} .

5.1 A free particle

Consider a massive particle that is free to move in one dimension. You are familiar with the quantum mechanical description of such system in terms of a (wave)function $\psi(x, t)$ and the Schroedinger equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, t) = i\hbar \frac{\partial}{\partial t} \psi(x, t) . \quad (5.2)$$

We can now see how this system fits the general framework described in the previous lectures: $\psi(x, t)$ is an element of a Hilbert space \mathcal{F} of functions (see the comment below if you are interested to know more about \mathcal{F}) with the scalar product defined in (2.6). The Hamiltonian is defined as

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} . \quad (5.3)$$

Let us re-interpret this description in terms of an abstract Hilbert space, where we have a position and a momentum operator satisfying

$$[\hat{x}, \hat{p}] \equiv \hat{x} \hat{p} - \hat{p} \hat{x} = i\hbar . \quad (5.4)$$

We use the symbol $|x_0\rangle$ to indicate the “generalized” eigenvectors of the position operator \hat{x} and $|\psi\rangle$ to indicate the ket representing the state of our system. The usual wavefunction represents nothing else than the coordinates of $|\psi\rangle$ along the basis $|x_0\rangle$

$$\psi(x_0) \equiv \langle x_0 | \psi \rangle . \quad (5.5)$$

In this basis we have

- The position operator \hat{x} is represented by the standard multiplication, that is the action of \hat{x} on the vector $|\psi\rangle$ correspond to multiply the wavefunction by x .
- Then from (5.4) we see the the momentum operator is $\hat{p} = -i\hbar \frac{\partial}{\partial x}$.
- $|x_0\rangle$ is represented by $\delta(x - x_0)$ (notice that this satisfies the normalization (3.8)).

Another very convenient basis is given by the (generalized) momentum eigenvectors $|p_0\rangle$. We know that in the position basis (that is when $\hat{p} = -i\hbar \frac{\partial}{\partial x}$) we have

$$\langle x | p_0 \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p_0 x} . \quad (5.6)$$

The factors in front has been chosen in order to satisfy the normalization condition (3.8). From (5.6) we see that the change from the coordinate basis to the momentum basis is nothing else but the Fourier transformation

$$\psi(x_0) = \int_{-\infty}^{\infty} \langle x_0 | p_0 \rangle \langle p_0 | \psi \rangle dp_0 = \int_{-\infty}^{\infty} e^{\frac{i}{\hbar} p_0 x_0} \psi(p_0) \frac{dp_0}{\sqrt{2\pi\hbar}}, \quad (5.7)$$

where we have defined $\langle p_0 | \psi \rangle \equiv \psi(p_0)$. The inverse relation expressing $\psi(p_0)$ in terms of $\psi(x_0)$ is simply

$$\psi(p_0) = \int_{-\infty}^{\infty} \langle p_0 | x_0 \rangle \langle x_0 | \psi \rangle dx_0 = \int_{-\infty}^{\infty} e^{\frac{-i}{\hbar} p_0 x_0} \psi(x_0) \frac{dx_0}{\sqrt{2\pi\hbar}}. \quad (5.8)$$

For the free particle the momentum basis is convenient because we know that the free Hamiltonian is $\hat{H} = \frac{\hat{p}^2}{2m}$ and this implies that \hat{H} and \hat{p} commute

$$[\hat{H}, \hat{p}] = 0. \quad (5.9)$$

Thus the eigenvectors (5.6) of \hat{p} are also eigenvectors of \hat{H} . Thus we can now write the time evolution of a generic vector $|\psi(t_0)\rangle$. We first write the state in the momentum basis and then use (5.1) to obtain

$$|\psi(t)\rangle = \int_{-\infty}^{\infty} e^{-\frac{ip^2}{2m\hbar}(t-t_0)} \psi(p, t_0) |p\rangle dp \quad (5.10)$$

Subtlety: The precise definition of \mathcal{F} is subtle somewhat subtle. Of course the functions in \mathcal{F} must be square integrable (the norm of the wavefunction should be finite) and, in order to show that this is really a Hilbert space, one needs to Lebesgue approach to defining the integrals. Moreover, consider two functions differ only in one point

$$f(x) = \frac{1}{1+x^2}, \quad g(x) = \begin{cases} \frac{1}{1+x^2} & \text{if } x \neq 0 \\ 0 & \text{if } x = 0 \end{cases} \quad (5.11)$$

Clearly we want to say that these two functions represent the same physical state, even if strictly speaking they are not equal. The “easiest” characterisation of \mathcal{F} is to start with the vector space discussed in the example 2.2.1 of *week 2* notes and consider its *completion*⁸. Mathematicians refer to this Hilbert space as $L^2(-\infty, \infty)$.

⁸This means that we add a new element to the vector space for each different Cauchy sequence which had no limit in the original vector space; in this way the requirement 2 in the definition of a Hilbert space is satisfied by construction.

5.1.1 Examples and exercises.

- Heisenberg uncertainty principle: by the triangular inequality and the commutation relation (5.4), we can derive Heisenberg's uncertainty principle. Let us suppose that the system (a massive particle in our case) is described by a $|\psi\rangle$. We can define the uncertainty on the measure of \hat{x} and \hat{p} as follows

$$(\Delta x)^2 = \langle \psi | (\hat{x} - x_a)^2 | \psi \rangle, (\Delta p)^2 = \langle \psi | (\hat{p} - p_a)^2 | \psi \rangle, \quad (5.12)$$

where x_a (p_a) are the average values of the position (momentum): $x_a = \langle \psi | \hat{x} | \psi \rangle$. We can see that $[(\hat{x} - x_a), (\hat{p} - p_a)] = [\hat{x}, \hat{p}]$. Thus by using (5.4) we see that $\langle \psi | [(\hat{x} - x_a), (\hat{p} - p_a)] | \psi \rangle = i\hbar$. Then

$$\begin{aligned} \hbar^2 &= |[(\hat{x} - x_a), (\hat{p} - p_a)]\psi|^2 = |\langle (\hat{x} - x_a)\psi | (\hat{p} - p_a)\psi \rangle - \langle (\hat{p} - p_a)\psi | (\hat{x} - x_a)\psi \rangle|^2 \\ &\leq |2\langle (\hat{x} - x_a)\psi | (\hat{p} - p_a)\psi \rangle|^2 \leq 4|\langle (\hat{x} - x_a)\psi | \psi \rangle|^2 |\langle (\hat{p} - p_a)\psi | \psi \rangle|^2. \end{aligned} \quad (5.13)$$

where in the last step I used Schwarz inequality (1.6).

- Consider a free particle of mass m . If a certain instant ($t = 0$) the particle is detected in $x = 0$ with an experimental uncertainty a . What's the probability of finding this particle at a distance at least y from the origin at the time t ? The approach you are probably familiar with is to write down Eq. (5.2) and try to find a solution for which⁹

$$\psi(x, t = 0) = \left(\frac{2}{\pi a^2} \right)^{\frac{1}{4}} e^{-\frac{x^2}{a^2}}. \quad (5.14)$$

(recall postulate 5!). The approach described in this paragraph suggests to use the momentum basis. In this basis we have

$$\begin{aligned} \psi(p, t = 0) &= \int_{-\infty}^{\infty} \langle p | x \rangle \langle x | p \rangle dx = \left(\frac{2}{\pi a^2} \right)^{\frac{1}{4}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{a^2} - \frac{i}{\hbar} px} \frac{dx}{\sqrt{2\pi\hbar}} \\ &= \left(\frac{a^2}{2\pi\hbar^2} \right)^{\frac{1}{4}} e^{-\frac{a^2 p^2}{4\hbar^2}}. \end{aligned} \quad (5.15)$$

Thus the evolved wavefunction in momentum space is

$$\psi(p, t) = \left(\frac{a^2}{2\pi\hbar^2} \right)^{\frac{1}{4}} e^{-\frac{ip^2 t}{2m\hbar} - \frac{a^2 p^2}{4\hbar^2}} \quad (5.16)$$

Now we can go back to position space where it is easier to compute the probability requested by the problem

$$\psi(x, t) = (2\pi a^2)^{\frac{1}{4}} \int_{-\infty}^{\infty} \exp\left(-\frac{ip^2 t}{2m\hbar} - \frac{a^2 p^2}{4\hbar^2} + \frac{ipx}{\hbar}\right) \frac{dp}{2\pi\hbar}. \quad (5.17)$$

⁹As usual, one can choose the overall constant A to work with a state of norm one: $A = (2\pi)^{1/4} \sqrt{a}$.

This is again a Gaussian integral and can be explicitly evaluated to find the wavefunction in the standard position space. The result takes exactly the same form of the $t = 0$ wavefunction (5.14), just with a time dependent parameter a !

$$\psi(x, t) = \left(\frac{2f(t)}{\pi a^2} \right)^{\frac{1}{4}} e^{-f(t) \frac{x^2}{a^2}}, \quad (5.18)$$

where $f(t)$ is a complex number and can be written as the product of its norm and phase or as the sum of the real and imaginary parts

$$f(t) = \frac{1}{1 + \frac{2i\hbar t}{a^2 m}} = \frac{e^{i\theta(t)}}{\sqrt{1 + \frac{4\hbar^2 t^2}{a^4 m^2}}} = \frac{1 - \frac{2m\hbar i t}{a^2 m^2}}{1 + \frac{4\hbar^2 t^2}{a^4 m^2}}. \quad (5.19)$$

So finally we can write the wavefunction at the time t and, in order to keep it as simple as possible, we summarize the overall phase in $\exp(i\Theta(t))$

$$\psi(x, t) = \left(\frac{2f(t)}{\pi a^2} \right)^{\frac{1}{4}} e^{i \frac{2m\hbar i t}{a^2 m^2} \frac{x^2}{a^2}} \exp \left(-\frac{x^2}{a^2 (1 + \frac{4\hbar^2 t^2}{a^4 m^2})} \right). \quad (5.20)$$

Notice that the probability density in position space is a Gaussian with a time dependent width

$$a(t) = \frac{a}{\sqrt{|f(t)|}} = a \sqrt{1 + \frac{4\hbar^2 t^2}{a^4 m^2}}. \quad (5.21)$$

So the uncertainty on the position of the particle increases over time. Since the average position is zero, we have

$$\Delta x^2 = \int_{-\infty}^{\infty} x^2 |\psi(x, t)|^2 dx = \frac{a^2}{4} \left(1 + \frac{4\hbar^2 t^2}{a^4 m^2} \right) \quad (5.22)$$

However the uncertainty over the momentum is constant! This is not immediately evident if we use the standard formulation

$$\Delta p^2 = \int_{-\infty}^{\infty} \psi(x, t)^* (-\hbar^2) \frac{d^2 \psi(x, t)}{dx^2} dx = \frac{\hbar^2}{a^2}, \quad (5.23)$$

but it is obvious if we use $\psi(p, t)$ in (5.16)

$$\Delta p^2 = \int_{-\infty}^{\infty} p^2 |\psi(p, t)|^2 dp = \int_{-\infty}^{\infty} p^2 |\psi(p, t=0)|^2 dp = \frac{\hbar^2}{a^2}. \quad (5.24)$$

Exercise. Consider a particle of mass m that is constrained to be in a 1-dimensional box of size $2a$, but that otherwise is free. For sake of concreteness, we will parametrize the box with $-a < x < a$.

- Find the eigenvectors and the eigenvalues of the Hamiltonian describing this system.
- At the time $t = 0$, the particle is described by the wavefunction $\psi(t = 0)$ which is in the positive half of the box ($0 < x < a$) with equal probability of being in any point of that part of the box. What is the probability of finding, in a physical measurement at the time $t = 0$, the lowest possible eigenvalue of the energy operator?
- Consider again the wavefunction $\psi(t = 0)$ described above: calculate the wavefunction at the time t supposing that it evolves freely (that is without any external perturbation).
- What is the probability of finding the particle in the negative half of the box at the time t ?
- What is the probability of finding, in a physical measurement at the time t , the lowest possible eigenvalue of the energy operator? What is the wavefunction describing the particle after this measurement?

5.2 The harmonic oscillator.

A particle of mass m moves in 1-dimension with a potential $U(x) = \frac{1}{2}kx^2$. The classical trajectory is an oscillatory motion with frequency ω

$$x(t) = A \cos(\omega t + \phi) , \quad \text{with } \omega = \sqrt{\frac{k}{m}} , \quad (5.25)$$

where ϕ is an arbitrary constant that we can set to zero by choosing an appropriate initial time $t = 0$ and A is the amplitude of the oscillation.

Quantum mechanically we know that the harmonic oscillator cannot have zero total energy, as this would violate Heisenberg's uncertainty principle. The state with minimal energy is called ground state and has energy $E_0 = \hbar\omega/2$. Then we have an infinite set of excited states with energies $E_n = \hbar\omega(n + 1/2)$. Let us derive these results by using an abstract operator description. The Hamiltonian of the system is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \quad (5.26)$$

and we want to find the eigenvectors of \hat{H} . The easiest approach is to consider the operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2m\hbar\omega}}\hat{p} , \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - i\sqrt{\frac{1}{2m\hbar\omega}}\hat{p} . \quad (5.27)$$

We can invert these relation and write the operators \hat{x} , \hat{p} in terms of the lowering and raising operators

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^\dagger) , \quad \hat{p} = -i\sqrt{\frac{m\hbar\omega}{2}} (\hat{a} - \hat{a}^\dagger) \quad (5.28)$$

In terms of the raising/lower operators the canonical commutation relations $[\hat{x}, \hat{p}] = i\hbar$ and the Hamiltonian (5.26) read

$$[\hat{a}, \hat{a}^\dagger] = 1 , \quad \hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \quad (5.29)$$

From this equation we immediately see that all energy eigenvalues must be positive. Suppose that $|\phi\rangle$ is an eigenvector of norm one and eigenvalue λ , then

$$\lambda = \langle \phi | \hat{H} | \phi \rangle = \hbar\omega \left(\langle \hat{a}\phi | \hat{a}\phi \rangle + \frac{1}{2} \right) > 0 . \quad (5.30)$$

An explicit realisation of the commutation relations in Eq. (5.29) is to think about the operators \hat{a} and \hat{a}^\dagger as acting on the space of polynomials $P(a)$ with complex coefficients: \hat{a} is identified with the derivative $\frac{d}{da}$ and so it lowers the degree of the polynomial by one, while \hat{a}^\dagger is identified with the multiplication by a and so raised the degree of the polynomial by one. We can easily check that this identification is consistent with the commutation relation

$$[\hat{a}, \hat{a}^\dagger] |v\rangle = |v\rangle \Leftrightarrow \frac{d}{da} (aP(a)) - a \frac{d}{da} (P(a)) = P(a) . \quad (5.31)$$

Then we need to define a scalar product on the space of polynomial such that the \hat{a} and \hat{a}^\dagger are actually one the adjoint of the other. Clearly this has to exchange the role of the multiplication by a and the derivative with the respect to a . So if each ket-vector is represented by standard polynomials (for instance $|P\rangle = a^2 + i$), the corresponding bra-vector is represented by the same polynomial where each a is substituted with a derivative and the new coefficients are the complex conjugate of the original one ($\langle P| = \frac{d^2}{da^2} - i$). The action of any bra on a vector is obtained simply by computing the action of the derivatives on the polynomial and then setting a to zero. So for instance, the scalar product of $|P\rangle$ and $|Q\rangle = a + 1$ is

$$\langle P | Q \rangle = \left[\left(\frac{d^2}{da^2} - i \right) (a + 1) \right]_{a=0} = \left[\frac{d^2 a}{da^2} + \frac{d^2 1}{da^2} - ia - i \right]_{a=0} = -i . \quad (5.32)$$

Now it is straightforward to check that the polynomial of degree zero $|0\rangle$ is the eigenstate of \hat{H} with minimal eigenvalue. In order for this to happen the first term on the right hand side of (5.30) should minimal possible value, *i.e.* zero:

$$\hat{a}|0\rangle = \left[\frac{d}{da} P(a) \right]_{a=0} = 0 \Rightarrow P(a) = \text{const} , \quad (5.33)$$

and so the corresponding eigenvalue of the harmonic oscillator Hamiltonian is $\hbar\omega/2$. By using the scalar product defined above we immediately see that the ground state as defined is normalised to one if we take $P(a) = 1$. Then it is clear that any other monomial $|n\rangle = C_n a^n$ is an eigenstate of the Hamiltonian in (5.29)

$$\hat{a}^\dagger \hat{a} |n\rangle = a \frac{d}{da} C_n a^n = n C_n a^n, \quad (5.34)$$

which implies that the corresponding eigenvalue for \hat{H} is

$$\lambda_n = \hbar\omega \left(n + \frac{1}{2} \right).$$

Again it is easy to fix the normalisation C_n by requiring

$$\langle n|n\rangle \Leftrightarrow |C_n|^2 \left[\frac{d^n}{da^n} a^n \right]_{a=0} = n! |C_n|^2, \quad (5.35)$$

which implies $C_n = 1/\sqrt{n!}$. Thus we can summarise the spectrum of \hat{H} by writing

$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n |0\rangle. \quad (5.36)$$

We saw that the operators \hat{a} and \hat{a}^\dagger lower/raise the energy level of an eigenstate of the Hamiltonian and that the normalised eigenvectors are related by

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \quad \text{and} \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \quad (5.37)$$

Finally a remark on the structure of the space of the possible states for the harmonic oscillator: the space of polynomials with the scalar product defined in (5.32) is not a Hilbert space, because it does not meet the second requirement listed at the end of Section 1. Thus we need to consider its completion, that is series, and not just polynomials, in a whose coefficients are square summable. So the full space of states is isomorphic to l^2 as defined in Section 1.

5.3 Connection with the usual wavefunctions.

Let us see that there is just a single state satisfying this condition. In order to do this, it is convenient to go back to the position space description $\psi_0(x) \equiv \langle x|0\rangle$, where the condition (5.33) reads as

$$\left(\sqrt{\frac{m\omega}{2\hbar}} x + \hbar \sqrt{\frac{1}{2m\hbar\omega}} \frac{d}{dx} \right) \psi_0(x) = 0. \quad (5.38)$$

This is a first order differential equation which has only one solution

$$\psi_0(x) = A \exp\left(-\frac{1}{2} \frac{m\omega}{\hbar} x^2\right) . \quad (5.39)$$

As usual, it is convenient to fix the overall normalization by requiring that the eigenstate has norm one, which implies

$$A = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} . \quad (5.40)$$

We can now use again the commutation relation (5.29) and build the entire spectrum of the harmonic oscillators (that is all the eigenvectors of \hat{H}) from the ground state by acting with \hat{a}^\dagger :

$$\hat{a}|0\rangle = 0 \Rightarrow \hat{N}(\hat{a}^\dagger)^n|0\rangle = n(\hat{a}^\dagger)^n|0\rangle . \quad (5.41)$$

This means that $(\hat{a}^\dagger)^n|0\rangle$ is proportional to $|n\rangle$; in particular, if we want to keep working with orthonormal eigenstates, we have

5.3.1 Examples and exercises.

Semiclassical states. The quantum mechanical energy eigenstates of the harmonic oscillator seems to be rather different from classic trajectories derived in (5.25). We would like to find a quantum mechanical state describing a motion that is very close to the classical one. In particular, we would like to find a state $|\alpha\rangle$ for which the *average* value of the position operator:

$$\langle\alpha|\hat{x}|\alpha\rangle = A \cos(\omega t + \phi) = \frac{1}{2} (Ae^{i\phi}e^{i\omega t} + Ae^{-i\phi}e^{-i\omega t}) . \quad (5.42)$$

By using (5.28), we can rewrite Eq. (5.42) as

$$\langle\alpha|\hat{x}|\alpha\rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle\alpha|\hat{a}\alpha\rangle + \sqrt{\frac{\hbar}{2m\omega}}\langle\alpha|\hat{a}^\dagger\alpha\rangle . \quad (5.43)$$

Clearly if we can find a ket that is an eigenstate of \hat{a} of eigenvalue

$$\alpha = \sqrt{\frac{m\omega}{2\hbar}}Ae^{-i\phi} ,$$

then (5.42) at $t = 0$ would follow. So let us look for a state $|\alpha\rangle$ satisfying

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle . \quad (5.44)$$

We can use the explicit realisation of the raising and lowering operators in (5.31) and transform (5.44) in a simple differential equation

$$\frac{d}{da}f(a) = \alpha f(a) \Rightarrow f(a) = \mathcal{A}e^{\alpha a} . \quad (5.45)$$

This function is not a polynomial, but can be approximated arbitrary well by a Cauchy series of polynomials, so it is part of the l^2 space describing the Harmonic oscillator states. Thus, in abstract terms, we see that the eigenstates we are looking for are

$$|\alpha\rangle = \mathcal{A}e^{\alpha\hat{a}^\dagger}|0\rangle. \quad (5.46)$$

These states are called coherent states and the average value for the position operator \hat{x} when the state of the particle is described by the coherent state α agrees with (5.42) for any t . We can check this explicitly by evolving $|\alpha\rangle$ at a generic time

$$|\alpha, t\rangle = e^{-\frac{i}{\hbar}Ht}|\alpha\rangle = \sum_{n=1}^{\infty} e^{-i\omega t(n+\frac{1}{2})} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \quad (5.47)$$

$$\begin{aligned} \langle\alpha, t|\hat{x}|\alpha, t\rangle &= |\mathcal{A}|^2 \sqrt{\frac{\hbar}{2m\omega}} \sum_{n,k=1}^{\infty} \frac{\bar{\alpha}^k \alpha^n}{\sqrt{k!n!}} (e^{i\omega t(k-n)} \langle k|a|n\rangle + e^{i\omega t(k-n)} \langle k|a^\dagger|n\rangle) \\ &= \frac{1}{2} (Ae^{i\phi}e^{i\omega t} + Ae^{-i\phi}e^{-i\omega t}). \end{aligned} \quad (5.48)$$

The second line follows from the first one by using (5.37), the result of the exercise below for \mathcal{A} and $\langle k|n\rangle = \delta_{kn}$ (recall that eigenstates with different eigenvalues are orthogonal).

Observation. There is a simpler way to derive (5.48) from (5.43). Suggestion: try to calculate the time derivative of $\langle\alpha, t|\hat{x}|\alpha, t\rangle$ by using (5.1).

Exercises.

- Normalize to one the coherent states (5.46).
- Consider a charged harmonic oscillator in a uniform constant electric field. Write the Hamiltonian and find the eigenvalues.

6 Perturbation theory.

We saw that finding the complete set of eigenvectors of the Hamiltonian is the key point to solve the dynamics of a physical system. Unfortunately it is often very difficult to solve exactly this problem. By now you have already seen the important situations where we can find all solutions to the eigenvector equation $H|\psi\rangle = E|\psi\rangle$

- The free particle and some simple variation where the potential is piecewise constant.
- The harmonic oscillator.