Lecture 4

Further developments

4.1 Introduction

In this lecture we are going to introduce some further concepts and general properties that are useful to describe simple quantum mechanical systems. We discuss how to deal with operators that have a *continuous* spectrum, and discuss some properties of expectation values and wave functions. We conclude the chapter by introducing briefly the Heisenberg representation, which is an alternative way to describe the time evolution of a quantum system.

4.2 Continuous spectrum

Until now we have discussed a number of examples where operators have a discrete spectrum, i.e. where the eigenvalues are numbered by some integer index k. [1] However there are operators that have a continuous spectrum, like e.g. the energy and the momentum of an unbound state, or the position operator $\hat{X}$. In order to deal with these cases, we need to generalize the formalism that we have introduced so far. As you will see below, the modifications are minimal, and rather straightforward.

4.2.1 Eigenvalue equation

Let us denote by $\hat{f}$ the operator associated to an observable with a continuous spectrum, the eigenvalue equation takes the form:

$$\hat{f}\psi_f(x) = f\psi_f(x), . \tag{4.1}$$

Once again, a generic state can be expanded as a superposition of eigenstates:

$$\psi(x) = \int df\, c(f)\psi_f(x)\,; \tag{4.2}$$

you should compare this expression with its analogue Eq. (2.18) in the case of discrete eigenvalues.

The coefficient of the expansion Eq. (4.2) is obtained by taking the scalar product:

$$c(f) = \langle f|\psi\rangle = \int dx\, \psi_f(x)^* \psi(x)\,. \tag{4.3}$$

The probabilistic interpretation of the wave function can be generalized:

> The probability of finding a result between f and $f+df$ for the observable $\hat{f}$ is given by:
> $$|c(f)|^2\, df\,.$$

[1] In the case of a discrete spectrum, the total number of eigenvalues may well be infinite, however the eigenvalues are labeled by integer numbers.

Thus we derive the normalization condition:

$$\int df\, |c(f)|^2 = 1\,. \tag{4.4}$$

4.2.2 Orthonormality

Following the steps performed to obtain Eq. (2.16), we have:

$$\int dx \psi_{f'}(x)^* \hat{f} \psi_f(x) = f \int dx \psi_{f'}(x)^* \psi_f(x)\,, \tag{4.5}$$

$$\int dx \psi_f(x)^* \hat{f} \psi_{f'}(x) = f' \int dx \psi_f(x)^* \psi_{f'}(x)\,. \tag{4.6}$$

Taking the complex conjugate of Eq. (4.5), and using the fact that $\hat{f}$ is Hermitean, yields:

$$\left(\int dx\, \psi_f(x)^* \hat{f} \psi_{f'}(x) \right)^* = \int dx\, \psi_{f'}(x)^* \hat{f}^\dagger \psi_f(x)\,, \tag{4.7}$$

$$= \int dx\, \psi_{f'}(x)^* \hat{f} \psi_f(x)\,. \tag{4.8}$$

Combining the results above:

$$\left(f - f'\right) \int dx\, \psi_{f'}(x)^* \hat{f} \psi_f(x) = 0\,, \tag{4.9}$$

and therefore, if $f \neq f'$,

$$\langle f' | f \rangle = 0\,. \tag{4.10}$$

Now comes a subtle point. The norm of the state $|\psi\rangle$ is given by:

$$\langle \psi | \psi \rangle = \int df\, df'\, c(f)^* c(f') \langle f | f' \rangle \tag{4.11}$$

$$= \int df\, |c(f)|^2 \int df' \langle f | f' \rangle\,, \tag{4.12}$$

where we used the orthogonality result Eq. (4.10). Now the integral over df' in Eq. (4.12) vanishes for any finite value of $\langle f | f \rangle$. Therefore we need to impose that $\langle f | f \rangle$ is infinite, and normalized so that

$$\int df'\, \langle f' | f \rangle = 1\,. \tag{4.13}$$

The *delta function* introduced by Dirac satisfies precisely this condition, so we can write:

$$\langle f' | f \rangle = \int dx\, \psi_{f'}(x)^* \psi_f(x)\,, \tag{4.14}$$

$$= \delta(f - f')\,. \tag{4.15}$$

Properties of the Dirac delta are summarized below.

4.2.3 Example: the free case

As an example of a system with a continuous spectrum we shall briefly recall the properties of the free quantum particle ($V = 0$). The Schrödinger equation reads:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)\,. \tag{4.16}$$

For $E > 0$ this equation has got two solutions:

$$u_{k,1}(x) = e^{ikx}, \quad u_{k,2}(x) = e^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}\,. \tag{4.17}$$

Each level (except for $E = 0$) is doubly degenerate, with the two solutions representing respectively particles travelling to the right and to the left. It is easy to check that the two eigenfunctions are also eigenfunctions of the momentum operator, and therefore correspond to states with momentum $\pm\hbar k$. Note that we have used two indices to identify the eigenfunctions: $k > 0$ is related to the value of the energy, and we can see that it spans a continuous spectrum. The second index is discrete, and runs from 1 to 2, simply to distinguish the two degenerate functions, *i.e.* the solution propagating to the right from the solution propagating to the left.

The time-dependent solution of Schrödinger equation reads:

$$\Psi_k(x,t) \equiv A\exp\{i(kx - \omega t)\} = A\exp\{i(px/\hbar - Et/\hbar)\}$$

which is an eigenfunction of both energy:

$$i\hbar\frac{\partial}{\partial t}\Psi_k(x,t) = \hbar\omega\Psi_k(x,t) \equiv E\Psi_k(x,t)$$

and momentum:

$$\hat{P}\Psi_k(x,t) = -i\hbar\frac{\partial}{\partial x}\Psi_k(x,t) = \hbar k\Psi_k(x,t) \equiv p\Psi_k(x,t)$$

and yet is not normalisable because

$$|\Psi_k(x,t)|^2 = |A|^2\exp\{i(kx - \omega t)\}\,\exp\{-i(kx - \omega t)\} = |A|^2$$

so that

$$\int_{-\infty}^{\infty} |\Psi_k(x,t)|^2\,dx = |A|^2\int_{-\infty}^{\infty} dx = \infty$$

However, the physical interpretation is obvious; we are equally likely to find the particle *anywhere* in the interval $-\infty < x < \infty$, so that the probability density is uniform. This can be regarded as a direct consequence of the Heisenberg uncertainty principle: the uncertainty in momentum is zero and therefore the uncertainty in position must be infinite.

We can circumvent this technical difficulty by, for example, pretending that we are dealing with a finite system and only taking the limit of an infinite system at the end of any computation.

Note that solutions with $E < 0$ yield a purely imaginary k, and therefore the eigenfunctions are not even bounded. Hence they do not represent physical states. The only allowed states for the free particle are the ones with positive (kinetic) energy.

We can now readily check that the eigenfunctions of the continuous spectrum found above satisfy the orthogonality and completeness relations discussed in Sects. 4.2.1, and 4.2.2:

$$\psi(x) = \int_0^\infty dk \, \left[\tilde{f}(k)e^{ikx} + \tilde{f}(-k)e^{-ikx}\right] , \tag{4.18}$$

$$\int dx \, e^{ix(k-k')} = 2\pi\delta(k-k') \, . \tag{4.19}$$

Eq. (4.18) is nothing but the well-known fact that normalizable functions admit a Fourier transfom. On the other hand Eq. (4.19) is a property of the Dirac delta, that you can find in the box below [2].

Note that Eq. (4.19) implies that the properly normalized eigenfunctions are:

$$u_{k,1}(x) = \frac{1}{\sqrt{2\pi}} \, e^{ikx}, \quad u_{k,2}(x) = \frac{1}{\sqrt{2\pi}} \, e^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \, . \tag{4.20}$$

[2] You will see again both these results in one of the Mathematics courses

Mathematical aside
The delta function is the natural extension of the familiar Kronecker delta δ_{ij} to the case of continuous variables; it is defined as:

$$\delta(x) = 0, \quad \text{if } x \neq 0, \qquad \delta(0) = \infty\,, \tag{4.21}$$

and

$$\int_a^b dx\, \delta(x) g(x) = \begin{cases} g(0), & \text{if } a < 0 < b\,, \\ 0, & \text{otherwise}\,, \end{cases} \tag{4.22}$$

for any continuous function $g(x)$.
The following properties are very useful when dealing with delta functions.

$$\int_a^b dx\, \delta(x-c) g(x) = \begin{cases} g(c), & \text{if } a < c < b\,, \\ 0, & \text{otherwise}\,; \end{cases} \tag{4.23}$$

$$\delta(-x) = \delta(x)\,; \tag{4.24}$$

$$\delta(ax) = \frac{1}{|a|}\delta(x)\,; \tag{4.25}$$

$$g(x)\delta(x-y) = g(y)\delta(x-y)\,; \tag{4.26}$$

$$x\delta(x) = 0\,; \tag{4.27}$$

$$\frac{d}{dx}\theta(x) = \delta(x)\,, \quad \text{where } \theta(x) = \begin{cases} 1, & \text{if } x \geq 0\,, \\ 0, & \text{if } x < 0\,; \end{cases} \tag{4.28}$$

$$\delta(g(x)) = \sum_{i=1}^{r} \frac{1}{|g'(x_i)|}\, \delta(x - x_i)\,, \quad \text{where } g(x_i) = 0\,; \tag{4.29}$$

$$\int_0^\infty dx\, g(x)\delta(x) = \frac{1}{2} g(0)\,. \tag{4.30}$$

The delta function can be defined as the limit of ordinary functions, here are some examples, that you are encouraged to sketch to visualize what happens.

$$\delta(x) = \lim_{\epsilon \to 0} \frac{1}{\sqrt{\pi}\epsilon} e^{-x^2/\epsilon^2}\,, \tag{4.31}$$

$$= \lim_{L \to \infty} \frac{\sin(Lx)}{\pi x}\,, \tag{4.32}$$

$$= \lim_{L \to \infty} \frac{\sin^2(Lx)}{\pi L x^2}\,, \tag{4.33}$$

$$= \lim_{\epsilon \to 0} \frac{1}{\pi} \frac{\epsilon}{\epsilon^2 + x^2}\,. \tag{4.34}$$

The folowing representation for the delta function is very useful:

$$\int_{-\infty}^{\infty} dx\, e^{ix(k-k')} = 2\pi\delta(k-k')\,. \tag{4.35}$$

4.2.4 Spectral decomposition

For a generic operator $\hat{O}$, the eigenvalue spectrum can be made of discrete eigenvalues O_n and continuous values f. In this case we need to consider both the eigenfunctions of the discrete spectrum and those of the continuos spectrum to have a basis to expand quantum states in.

$$\psi(x) = \sum_n c_n \psi_n(x) + \int df\, c(f)\psi_f(x) \tag{4.36}$$

$$|\psi\rangle = \sum_n \langle n|\psi\rangle\, |n\rangle + \int df\, \langle f|\psi\rangle\, |f\rangle\,. \tag{4.37}$$

Eq. (4.36) summarizes the completeness relation for both discrete and continuous spectra.

4.3 General properties

There are some nice theorems that can be *derived* from the postulates of the theory. They are logical consequences of the principles that we have set up, and do not require further assumptions. They yield further information on the dynamics of the systems that we wish to study.

4.3.1 Energy expectation value

The expectation value of the energy in a quantum state is given by:

$$\langle\Psi|\hat{H}|\Psi\rangle = \int dx\, \Psi(x,t)^* \left(\frac{\hat{P}^2}{2m} + \hat{V}\right)\Psi(x,t) \tag{4.38}$$

$$= -\frac{\hbar^2}{2m}\int dx\, \Psi(x,t)^* \frac{d^2}{dx^2}\Psi(x,t) + \int dx\, \Psi(x,t)^* V(x)\Psi(x,t) \tag{4.39}$$

$$= \frac{\hbar^2}{2m}\int dx\, \left|\frac{d}{dx}\Psi(x,t)\right|^2 + \int dx\, V(x)\, |\Psi(x,t)|^2 \tag{4.40}$$

$$\geq V_{\min}\int dx\, |\Psi(x,t)|^2 = V_{\min}\,, \tag{4.41}$$

i.e. the expectation value of the energy is always larger than the minimum of the potential energy:

$$\boxed{\langle E\rangle \geq V_{\mathrm{min}}}\,. \tag{4.42}$$

4.3.2 Ehrenfest's theorem

Using Eq. (3.39) the following equations can be proved:

$$\frac{d}{dt}\langle m\hat{X}\rangle = \langle \hat{P}\rangle\,, \tag{4.43}$$

$$\frac{d}{dt}\langle \hat{P}\rangle = -\langle \frac{d}{dX} V(\hat{X})\rangle\,. \tag{4.44}$$

This result is known as Ehrenfest's theorem. It is interesting to note that the expectation values of the position and momentum operators satisfy the same equations of motion that we find in Newtonian mechanics. Eq. (4.43) is easily proven using the fact that $\left[m\hat{X}, \hat{P}^2/(2m)\right] = i\hbar\hat{P}$. In order to obtain Eq. (4.44) you need to use the following relation:

$$\left[\hat{P}, V(\hat{X})\right] = -i\hbar\frac{d}{dX}V(\hat{X})\,, \tag{4.45}$$

where $(d/dx)V$ denotes the derivative of V with respect to its argument.

4.3.3 Degeneracy and oscillations

The results in Secs. 4.3.1, and 4.3.2 apply to systems in any number of dimensions. The following results instead are only valid for one-dimensional systems.

The discrete energy levels in a one-dimensional potential well are not degenerate.

Proof. Let us assume the contrary, namely that there is an energy value E for which we have two degenerate eigenstates ψ_1 and ψ_2. The two eigenfunctions satisfy the same equation:

$$\psi_1'' = -\frac{2m}{\hbar^2}\left(E - V(x)\right)\psi_1\,, \tag{4.46}$$

$$\psi_2'' = -\frac{2m}{\hbar^2}\left(E - V(x)\right)\psi_2\,. \tag{4.47}$$

Multiplying the first equation by ψ_2 and the second one by ψ_1, and subtracting them, we obtain:

$$\psi_2\psi_1'' - \psi_1\psi_2'' = 0\,. \tag{4.48}$$

Integrating with respect to x yields:

$$\psi_1'(x)\psi_2(x) - \psi_2'(x)\psi_1(x) = \text{const}\,. \tag{4.49}$$

Since the eigenstates must be normalizable, we deduce that $\psi_1 = \psi_2 = 0$ at $x = +\infty$, and hence const $= 0$,

$$\psi_1'(x)\psi_2(x) - \psi_2'(x)\psi_1(x) = 0\,. \tag{4.50}$$

Integrating again with respect to x:

$$\log\psi_1 = \log\psi_2 + \text{const}\,, \tag{4.51}$$

i.e. ψ_1 and ψ_2 are proportional and therefore describe the *same* eigenstate, which contradicts the initial statement.

The second theorem states that

The wave function of the n-th discrete energy level has $n-1$ zeroes.

In particular, the wave function of the ground state does not vanish, for any value of x.

We shall not prove this theorem explicitly.

4.4 Heisenberg representation

Let us conclude this lecture by discussing a different way to characterize the time evolution of a quantum system.

In the Schrödinger picture the state of the system evolves in time, while the operators are usually time-independent. The expectation value of an observable O at time t is given by:

$$\langle\Psi(t)|\hat{O}|\Psi(t)\rangle = \langle\Psi(0)|e^{i\hat{H}t/\hbar}\hat{O}e^{-i\hat{H}t/\hbar}|\Psi(0)\rangle\,, \tag{4.52}$$

where we have used Eq. (3.17) to express $|\Psi(t)\rangle$ as a function of $|\Psi(0)\rangle$.

We can now interpret Eq. (4.52) as the expectation value of a time-dependent observable:

$$\boxed{\hat{O}_H(t) = e^{i\hat{H}t/\hbar}\hat{O}e^{-i\hat{H}t/\hbar}}\,, \tag{4.53}$$

whose expectation is computed between time-independent states. This is called the *Heisenberg representation.*

The dynamics in the Heisenberg representation is dictated by an equation describing the time evolution of the operators:

$$i\hbar\frac{d}{dt}\hat{O}_H(t) = \left[\hat{O}_H, \hat{H}\right]\,. \tag{4.54}$$

Depending on the problem that you are trying to solve, one representation may be more effective than the other. The physical predictions however must be identical!

4.5 Summary

As usual, we summarize the main concepts introduced in this lecture.

- Completeness and orthogonality relations for the continuous spectrum.
- Free particle as an example of the above concepts.
- More properties of the solutions of Schrödinger equation.
- The Heisenberg representation.