Lecture 7

More dimensions

7.1 Introduction

In this lecture we generalize the concepts introduced so far to systems that evolve in more than one spatial dimension. While the generalization of the concepts is straightforward, we will encounter new features that were not present for one-dimensional systems. The three-dimensional formulation will allow us to discuss more realistic examples.

7.2 Quantum states

We discuss here the case of three spatial dimensions; positions in space are specified by e.g. threee Cartesian coordinates (x, y, z). All results can be reduced to the case of a two-dimensional space by dropping the dependence on the third coordinate z.

As in the one-dimensional case, quantum states are described by a wave function - cfr Eq. (1.5):

$$\boxed{\text{quantum state} \sim \Psi(\underline{r}, t)\,,} \tag{7.1}$$

the wave function is now a function of the position vector: $\underline{r}$. After choosing a reference frame in space, the vector is uniquely idetified by its coordinates (x, y, z) in that reference frame.

The modulo square of the wave function has the same probabilistic interpretation discussed in Lecture 1:

> $|\Psi(\underline{r}, t)|^2\, d\tau$ is the probability that a measurement of the position of the particle yields a result in the infinitesimal volume element $d\tau$ at $\underline{r}$ with $d\tau = dx\, dy\, dz$ in Cartesian coordinates or $r^2 \sin\theta\, dr\, d\theta\, d\phi$ in spherical polars.

Thus $|\Psi(\underline{r}, t)|^2$ is a *probability per unit volume*.
The normalisation condition becomes

$$\int_{\text{all space}} d\tau\, |\Psi(\underline{r}, t)|^2 = 1\,. \tag{7.2}$$

The physical meaning of this equation should be clear: the probability of finding the system *somewhere* in space must be equal to one.

Note that if the system under consideration is a two-dimensional system, then the position vector is a two-dimensional Euclidean vector, and all the integrals are computed over two-dimensional surfaces.

We can still use Dirac's notation to denote a state vector:

$$\Psi(\underline{r}, t) \longleftrightarrow |\Psi(t)\rangle\,. \tag{7.3}$$

The scalar product of two states now involves an integral over the whole volume:

$$\langle \Phi(t')|\Psi(t)\rangle = \int d\tau\, \Phi(\underline{r}, t')^* \Psi(\underline{r}, t), . \tag{7.4}$$

The normalization condition in Dirac's notation is:

$$\langle \Psi|\Psi\rangle = 1\,. \tag{7.5}$$

Note that, when using Dirac's notation, the condition is written exactly in the same form in any number of dimensions. However the meaning of the scalar product denoted by the bra and ket notation is different as we vary the number of dimensions - the integral in the scalar product extends over the whole spatial volume.

7.3 Observables

As far as observables are concerned, there is no conceptual difference between the one-dimensional systems that we discussed in the first part of the lectures, and systems in higher-dimensional spaces. Observables are in one-to-one correspondence with linear Hermitean operators acting on the wave functions.

Let us summarize the main features of the correspondence:

- The eigenvalues of the operator $\hat{O}$ yield the possible outcomes of a measurement of the observable O.
- You can easily check that the orthogonality relations that we proved for the eigenfunction of a Hermitean operator in the one-dimensional case are still true.
- Likewise, the set of eigenfunctions of a Hermitean operator are a *complete* set and therefore any wave function can be expanded using these eigenfunctions as basis.

A quantum state can be expanded:

$$|\psi\rangle = \sum_n c_n |\psi_n\rangle\,.$$

The eigenstates $|\psi_n\rangle$ are the basis vectors, and the coefficients c_n are the coordinates. As we discussed earlier in this course, the vector space in quantum mechanics is a complex space, and therefore the coefficients c_n are complex.

Example The eigenvalue equation for a Hermitean operator $\hat{O}$ in a three-dimensional system is:

$$\hat{O}\psi_k(\underline{r}) = O_k\psi_k(\underline{r})\,. \tag{7.6}$$

Note that in this case the eigenfunctions depend on the vector $\underline{r}$. This is the only peculiarity of the three-dimensional case. The eigenvalues O_k are the possible values for O, the eigenfunctions $\psi_k(\underline{r})$ describe quantum states where a measurement of O would yield O_k with probability one.

The completeness of the eigenfunctions is expressed by the fact:

$$\psi(\underline{r}) = \sum_k c_k\psi_k(\underline{r})\,, \tag{7.7}$$

for any generic quantum state $\psi(\underline{r})$. As before, $|c_k|^2$ yields the probability of getting the value O_k upon measuring O in the state ψ. The coefficients c_k are obtained from the scalar products:

$$c_k = \langle\psi_k|\psi\rangle\,, \tag{7.8}$$

where now the scalar product requires a three-dimensional integral, according to Eq. (7.4).

Using Dirac's notation, the definition of the Hermitean conjugate is formally unchanged:

$$\langle\phi|\hat{O}^\dagger|\psi\rangle = \Big(\langle\psi|\hat{O}|\phi\rangle\Big)^*\,. \tag{7.9}$$

If you want to rewrite the relation above using wave functions and integrals, you get:

$$\int d\tau\,\phi(\underline{r})^*\hat{O}^\dagger\psi(\underline{r}) = \left(\int d\tau\,\psi(\underline{r})^*\hat{O}\phi(\underline{r})\right)^*\,. \tag{7.10}$$

Remember that now we need to integrate over three-dimensional space, $d\tau$ is the infinitesimal integration volume.

Example It is interesting to consider the generalization of the momentum operator defined in Eq. (2.30) for the one-dimensional system. The momentum is a three-dimensional vector $\underline{P}$ which can be represented by its three components in a Cartesian reference frame (P_x, P_y, P_z). Following our general prescription, to each component of the momentum we associate a Hermitean operator:

$$\hat{P}_x = -i\hbar\frac{\partial}{\partial x}\,, \tag{7.11}$$

$$\hat{P}_y = -i\hbar\frac{\partial}{\partial y}\,, \tag{7.12}$$

$$\hat{P}_z = -i\hbar\frac{\partial}{\partial z}\,. \tag{7.13}$$

Hence for instance:

$$\hat{P}_x\psi(\underline{r}) = -i\hbar \left.\frac{\partial\psi}{\partial x}\right|_{\underline{r}} . \tag{7.14}$$

A concise notation for the momentum operator is :

$$\underline{\hat{P}} = -i\hbar\underline{\nabla} . \tag{7.15}$$

We shall use the notation x_i, with $i = 1, 2, 3$ to denote the three components x, y, z respectively. Similarly $\frac{\partial}{\partial x_i}$ will be used to indicate $\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}$ respectively. Using a simple property of partial derivatives, we have:

$$\hat{P}_i\hat{P}_j\psi(\underline{r}) = -\hbar^2\frac{\partial^2}{\partial x_i\partial x_j}\psi(\underline{r}) = -\hbar^2\frac{\partial^2}{\partial x_j\partial x_i}\psi(\underline{r}) = \hat{P}_j\hat{P}_i\psi(\underline{r}) . \tag{7.16}$$

Different components of the momentum commute with each other, i.e. they can all be measured simultaneously.

Following the derivation that led to Eq. (2.41), you can readily prove the canonical commutation relations in three dimensions:

$$\left[\hat{X}_i, \hat{P}_j\right] = i\hbar\delta_{ij} . \tag{7.17}$$

Thus $\hat{X}$ *does not* commute with $\hat{P}_x$, but *does* commute with $\hat{P}_y$ and $\hat{P}_z$. These commutation relations lead to Heisenberg uncertainty relations involving the components of the position and the momentum of the particle:

$$\Delta X_i \cdot \Delta P_j \geq \frac{\hbar}{2}\delta_{ij} . \tag{7.18}$$

7.4 Dynamics

Similarly to the case of one-dimensional systems, the dynamics is determined by the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(\underline{r}, t) = \hat{H}\Psi(\underline{r}, t) . \tag{7.19}$$

In three dimensions the hamiltonian for the system can be expressed as:

$$\begin{aligned} \hat{H} &= \hat{T} + \hat{V} \\ &= -\frac{\hbar^2}{2m}\nabla^2 + V(\underline{\hat{X}}) , \end{aligned} \tag{7.20}$$

where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{7.21}$$

is the Laplace operator. Thus the time evolution of a quantum state is found by solving the differential equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(\underline{r},t) = \left\{-\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r})\right\}\Psi(\underline{r},t)\,. \tag{7.22}$$

As in the one-dimensional case, we are going to solve the time-dependent Schrödinger equation by expanding the solution in eigenstates of the Hamiltonian. The latter are obtained by solving the eigenvalue problem for $\hat{H}$, i.e. the time-independent Schroödinger equation:

$$\hat{H}\psi_E(\underline{r}) = E\psi(\underline{r})\,. \tag{7.23}$$

Example Let us discuss the solution of the time-independent Schrödinger equation for the isotropic harmonic oscillator in 3 dimensions, for which the potential is

$$V(\underline{r}) = \tfrac{1}{2}m\omega^2 r^2 = \tfrac{1}{2}m\omega^2\left(x^2+y^2+z^2\right) \tag{7.24}$$

The eigenvalue problem can be separated in Cartesian coordinates by writing:

$$u_n(\underline{r}) = X(x)\cdot Y(y)\cdot Z(z)\,, \tag{7.25}$$

yielding

$$\left\{-\frac{\hbar^2}{2m}\,\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{2}m\omega^2x^2\right\}+\left\{-\frac{\hbar^2}{2m}\,\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{1}{2}m\omega^2y^2\right\}+\left\{-\frac{\hbar^2}{2m}\,\frac{1}{Z}\frac{d^2Z}{dz^2}+\frac{1}{2}m\omega^2z^2\right\} = E_n\,. \tag{7.26}$$

Each term in braces must be equal to a constant, so we can write

$$E_{n_x}+E_{n_y}+E_{n_z} = E_n \tag{7.27}$$

with, for example,

$$\left\{-\frac{\hbar^2}{2m}\,\frac{d^2X}{dx^2}+\tfrac{1}{2}m\omega^2x^2\,X\right\} = E_{n_x}X\,, \tag{7.28}$$

which is just a 1-dimensional oscillator problem for which we know the solution:

$$E_{n_x} = \left(n_x+\tfrac{1}{2}\right)\hbar\omega\,,\quad n_x = 0,\,1,\,2,\,3\ldots \tag{7.29}$$

$$X(x) = u_{n_x}(x) = C_{n_x}\,\exp(-\alpha^2x^2/2)\,H_{n_x}(\alpha x)\,. \tag{7.30}$$

Thus

$$E_n = \left(n_x+n_y+n_z+\tfrac{3}{2}\right)\hbar\omega,\quad n_x,n_y,n_z = 0,\,1,\,2,\,3\ldots \tag{7.31}$$

$$\equiv \left(n+\tfrac{3}{2}\right)\hbar\omega,\quad n = 0,\,1,\,2,\,3\ldots \tag{7.32}$$

7.5 Degeneracy

We see in the previous example a new feature, that we had not encountered in the one-dimensional case. The three-dimensional harmonic oscillator displays *degeneracy*, i.e. more than one eigenfunction correspond to the *same* eigenvalue.

Eq. (7.31) shows that a given value of E_n can arise in more than one way. For example:

n	n_x	n_y	n_z	g_n
0	0	0	0	1
	1	0	0	
1	0	1	0	3
	0	0	1	

g_n is the number of ways that a given value of n, and hence of the energy E_n, can arise, and is called the *degree of degeneracy*. We say, for example, that the $n = 1$ level is 3-fold degenerate, meaning that there are three distinct quantum states of the same energy, corresponding to the eigenfunctions

$$u_1(x) \cdot u_0(y) \cdot u_0(z), \quad u_0(x) \cdot u_1(y) \cdot u_0(z), \quad u_0(x) \cdot u_0(y) \cdot u_1(z)\,. \tag{7.33}$$

7.6 Summary

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

- Description of three-dimensional quantum states.
- Implementation of the observables as Hermitean operators.
- Momentum operator and commutation relations.
- Schrödinger equation, stationary states and separation of variables.
- Degeneracy.