Lecture 10 – Uncertainty principles and conserved quantities

MATH-GA 2710.001 Mechanics

1 Dirac's notation

We will introduce here a very convenient notation to handle operator algebra in quantum mechanics. The notation was pioneered in a large part by the British physicist Paul Dirac. Beyond its convenience, it has the major advantage that it remains the same independently of the representation one chooses.

1.1 State vectors: "kets" and "bras"

We have seen two possible representations for a quantum systems: the "**r** representation" and the "**p** representation". There are many other possible representations, and in many cases the **r** and **p** representations are not the most convenient to use. Let us therefore consider the quantum state ψ as an element in some given abstract Hilbert space $\mathcal{E}$, and write it with a vertical bar on its left and the symbol $\rangle$ on its right: $|\psi\rangle$. $|\psi\rangle$ is called the "ket" ψ. The reason for this notation will soon be very clear. ψ could be $\Psi(\mathbf{r}, t)$ in "**r** representation", $\Phi(\mathbf{p}, t)$ in "**p** representation", or the column vector **c** in a discrete representation as we have seen in Lecture 9.

The inner product we have seen in the previous lecture is put in the following formal framework:

- to each ket $|\chi\rangle$ in $\mathcal{E}$ we associate a *linear functional* (also called *one-form*) that belongs to the dual space $\mathcal{E}^*$ and which we write $\langle\chi|$. Such an element of $\mathcal{E}^*$ is (somewhat abusively) called a "bra" vector. When one applies this one-form to any ket $|\psi\rangle$ one obtains a complex number that can be seen as an inner product which is written $\langle\chi|\psi\rangle$. The justification for the notation and the names "bra" and "ket" becomes more transparent at this point.
- The correspondence $|\psi\rangle \;\rightarrow\; \langle\psi|$ is antilinear:

$$\lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle \;\rightarrow\; \lambda_1^*\langle\psi_1| + \lambda_2^*\langle\psi_2|$$

- The inner product satisfies the properties:
  1. Linearity with respect to the kets and antilinearity with respect to the bras
  2. $(\langle\chi|\psi\rangle)^* = \langle\psi|\chi\rangle$
  3. $\langle\psi|\psi\rangle \geq 0$, and equality is only true if $|\psi\rangle$ is the null ket vector.

1.2 Operator conventions

Although operators have a different expression depending on the representation that is chosen, the commutation relations between operators are independent of the representation. In Dirac's formalism, the order in which the operators have to be written and to be applied to the bra vectors and the ket vectors is determined independently of the representation in which these operators are written:

- The ket that is obtained by applying the operator $\widehat{O}$ to the ket $|\psi\rangle$ is written $\widehat{O}|\psi\rangle$. In other words, the operator is written on the left of the ket. If one applies successively $\widehat{O}_1$, $\widehat{O}_2$, and then $\widehat{O}_3$ to $|\psi\rangle$, the resulting ket is written

$$\widehat{O}_3\widehat{O}_2\widehat{O}_1|\psi\rangle$$

- The bra that us obtained by applying the operator $\widehat{O}$ to the bra $\langle\psi|$ is $\langle\psi|\widehat{O}$: the operator is written to the right of the bra. If one applies successively $\widehat{O}_1$, $\widehat{O}_2$, and then $\widehat{O}_3$ to $\langle\psi|$, one writes

$$\langle\psi|\widehat{O}_1\widehat{O}_2\widehat{O}_3$$

With these conventions, you can convince yourself that the bra associated with the ket $\widehat{O}|\psi\rangle$ is $\langle\psi|\widehat{O}^\dagger$, where $\widehat{O}^\dagger$ is the Hermitian conjugate of $\widehat{O}$. You can see this by translating this in the **r** representation. Conversely, the ket associated with $\langle\psi|\widehat{O}$ is $\widehat{O}^\dagger|\psi\rangle$. In this context, the inner product that we used to write

$$\langle\chi(\mathbf{r}), \widehat{O}\Psi(\mathbf{r})\rangle = \langle\widehat{O}^\dagger\chi(\mathbf{r}), \Psi(\mathbf{r})\rangle$$

in **r** representation can now be written

$$\langle\chi|(\widehat{O}|\psi\rangle) = (\langle\chi|\widehat{O})|\psi\rangle$$

We see that the parentheses are not necessary above, so we will simply write

$$\langle\chi|\widehat{O}|\psi\rangle$$

One may at this point start to see the advantage of using Dirac's notation. Let us continue in this vein. The expression

$$\langle\chi|\widehat{O}_2\widehat{O}_1|\psi\rangle$$

can be computed in several ways: we can see it as the inner product of the bra $\langle\chi|$ with the ket $\widehat{O}_2\widehat{O}_1|\psi\rangle$, or as the inner product of the bra $\langle\chi|\widehat{O}_2$ with the ket $\widehat{O}_1|\psi\rangle$ (which would be $\langle\widehat{O}_2^\dagger\chi(\mathbf{r}),\widehat{O}_1\Psi(\mathbf{r})\rangle$ in $\mathbf{r}$ representation), or as the inner product with the bra $\langle\chi|\widehat{O}_2\widehat{O}_1$ with the ket $|\psi\rangle$ ($\langle\widehat{O}_1^\dagger\widehat{O}_2^\dagger\chi(\mathbf{r}),\Psi(\mathbf{r})\rangle$ in $\mathbf{r}$ representation).

Wth the conventions introduced above, one can also see that the norm of the ket $\widehat{O}|\psi\rangle$ is written $\langle\psi|\widehat{O}^\dagger\widehat{O}|\psi\rangle$. And the following holds

$$(\langle\chi|\widehat{O}|\psi\rangle)^* = \langle\psi|\widehat{O}^\dagger|\chi\rangle$$

For Hermitian operators, many of the formulae above take a particularly simple form.

1.3 Discrete representations and matrix representations of operators

We focus here on the particular yet important situation in which the quantum states belong to a finite dimensional subspace $\mathcal{S}$ with dimension N of the Hilbert space. In this subspace, let us consider an orthonormal basis of N vectors written as kets $|\alpha\rangle$. Any ket vector $|\psi\rangle$ in $\mathcal{S}$ can then be expanded as

$$|\psi\rangle = \sum_{i=1}^{N} c_\alpha|\alpha\rangle$$

where the c_α are complex numbers given by

$$c_\alpha = \langle\alpha|\psi\rangle$$

In quantum mechanics, we therefore often write the expansion of ψ as follows

$$|\psi\rangle = \sum_{\alpha=1}^{N} |\alpha\rangle\langle\alpha|\psi\rangle$$

The state of the system is fully determined by the knowledge of the column vector $(c_\alpha)_{\alpha=1,\ldots,N}$. The operator $\widehat{A}$ of a physical observable can be fully characterized by looking at the way the operator acts on the kets of the orthonormal basis. Let $|\beta\rangle$ be one such ket. $\widehat{A}|\beta\rangle$ is a ket that can be expanded on the orthonormal basis:

$$\widehat{A}|\beta\rangle = \sum_{\alpha=1}^{N} |\alpha\rangle\langle\alpha|\widehat{A}|\beta\rangle$$

In other words, $\widehat{A}|\beta\rangle$ is a column vector whose αth component is $A_{\alpha\beta} \equiv \langle\alpha|\widehat{A}|\beta\rangle$. The knowledge of the $A_{\alpha\beta}$ for all α and β is clearly sufficient to determine the result of applying the operating $\widehat{A}$ to any ket $|\psi\rangle$. If we call $|\chi\rangle$ the ket $\widehat{A}|\psi\rangle$, we have

$$|\chi\rangle = \widehat{A}|\psi\rangle = \sum_{\beta=1}^{N} c_\beta\widehat{A}|\beta\rangle = \sum_{\beta=1}^{N} c_\beta\left(\sum_{\alpha=1}^{N} A_{\alpha\beta}|\alpha\rangle\right) = \sum_{\alpha=1}^{N}\left(\sum_{\beta=1}^{N} A_{\alpha\beta}c_\beta\right)|\alpha\rangle$$

In other words, the operator $\widehat{A}$ acts like a matrix whose elements are given by $A_{\alpha\beta} = \langle\alpha|\widehat{A}|\beta\rangle$. This is the reason why any expression of the form $\langle\alpha|\widehat{A}|\beta\rangle$ is often called a *matrix element* in quantum mechanics.

To go from $\widehat{A}$ in the $\mathbf{r}$ representation to its matrix representation in the discrete representation, one uses the fact that the inner product is independent of the representation with which one computes it. We thus use the known expression for $\widehat{A}$ in the $\mathbf{r}$ representation, and take the functions $\phi_\alpha(\mathbf{r})$ associated with the kets $|\alpha\rangle$ of the finite dimensional basis to compute

$$A_{\alpha\beta} = \langle\phi_{\alpha(\mathbf{r})},\widehat{A}\phi_b(\mathbf{r})\rangle = \int \phi_\alpha^*(\mathbf{r})\widehat{A}\phi_\beta(\mathbf{r})d\mathbf{r}$$

We have illustrated here the fact that there are two complementary ways of formulating quantum mechanics: 1) a "wave mechanics" picture, championed by Schrödinger and de Broglie (among others), and the one we had seen thus far with the **r** and **p** representations of operators; 2) a "matrix mechanics" picture, championed by Heisenberg, Born and Jordan among others, which we have just introduced here. Loosely speaking, in the "wave mechanics" picture, the operators are fixed, but the state vectors evolve in time. In the "matrix mechanics" picture the state vectors remain fixed, but the operator matrices are time dependent. Historically, the Schödinger picture came after the Heisenberg picture. Both have been shown to be equivalent, but you will likely still hear famous people giving arguments in favor of one or the other. It is mostly a matter of taste.

2 Physical meaning of commutation relations between operators

2.1 Compatible observables

If two observable physical quantities A and B can be simultaneously observed, then the associated operators $\widehat{A}$ and $\widehat{B}$ must have a common basis of eigenfunctions. We say that A and B are compatible. Let us call $|a_m, b_n, (l)\rangle$ the ket eigenfunctions associated with the eigenvalue a_m of $\widehat{A}$ and the eigenvalue b_n of $\widehat{B}$. The index (l) is to remind the reader that there may be orthonormal eigenfunctions that share an eigenvalue. As we just said, A and B are compatible if for any ket $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_{m,n,(l)} c_{m,n,(l)} |a_m, b_n, (l)\rangle$$

We now successively apply $\widehat{A}$ and $\widehat{B}$ to $|\psi\rangle$:

$$\widehat{A}|\psi\rangle = \sum_{m,n,(l)} c_{m,n,(l)} a_m |a_m, b_n, (l)\rangle$$
$$\Rightarrow \ \widehat{B}(\widehat{A}|\psi\rangle) = \sum_{m,n,(l)} c_{m,n,(l)} a_m b_n |a_m, b_n, (l)\rangle$$

Since scalar multiplication is commutative, it is clear that

$$\widehat{B}(\widehat{A}|\psi\rangle) = \sum_{m,n,(l)} c_{m,n,(l)} a_m b_n |a_m, b_n, (l)\rangle = \widehat{B}(\widehat{A}|\psi\rangle) = \sum_{m,n,(l)} c_{m,n,(l)} b_n a_m |a_m, b_n, (l)\rangle = \widehat{A}(\widehat{B}|\psi\rangle)$$

Since this is true for any ket $|\psi\rangle$,

$$\left[\widehat{A}, \widehat{B}\right] = 0$$

In other words, a necessary condition for two observables to be compatible is that their associated operators commute. We will soon see that this is also a sufficient condition.

2.2 Heisenberg's inequality

We just showed that if the commutator of two operators $\widehat{A}$ and $\widehat{B}$ is not zero, the associated physical quantities are incompatible. In particular, we will now show that if the following holds

$$\left[\widehat{A}, \widehat{B}\right] = i\hbar$$

then the physical quantities A and B satisfy Heisenberg's uncertainty principle

$$\Delta A \Delta B \geq \frac{\hbar}{2} \tag{1}$$

where ΔA is the standard deviation of the distribution of A, which is the square root of the variance.

We start by shifting the distributions so that the resulting distributions have zero mean. This corresponds to the following shift for the associated operators:

$$\widehat{A}' = \widehat{A} - \overline{A}\widehat{I} \qquad \widehat{B}' = \widehat{B} - \overline{B}\widehat{I}$$

where $\widehat{I}$ is the identity operator. This shift did clearly not change the variance, so we have

$$\Delta A'^2 = \overline{A'^2} = \Delta A^2$$
$$\Delta B'^2 = \overline{B'^2} = \Delta B^2$$

Furthermore,

$$[\widehat{A}', \widehat{B}'] = [\widehat{A}, \widehat{B}]$$

since all operators commute with $\widehat{I}$. Now, we can evaluate

$$\Delta A^2 = \Delta A'^2 = \overline{A'^2} = \langle\psi|\widehat{A}'^2|\psi\rangle = \langle\psi|\widehat{A}'\widehat{A}'|\psi\rangle$$
$$\Delta B^2 = \Delta B'^2 = \overline{B'^2} = \langle\psi|\widehat{B}'^2|\psi\rangle = \langle\psi|\widehat{B}'\widehat{B}'|\psi\rangle$$

Since $\widehat{A}$ and $\widehat{B}$ are Hermitian, $\langle\psi\widehat{A}'\widehat{A}'|\psi\rangle$ and $\langle\psi\widehat{B}'\widehat{B}'|\psi\rangle$ are the norms of $\widehat{A}|\psi\rangle$ and $\widehat{B}|\psi\rangle$ respectively. Therefore, the quantity $\Delta A^2 \Delta B^2$ is the product of two norms. By the Cauchy-Schwarz inequality, we know that this product is greater than or equal to square of the inner product of the two vectors:

$$\Delta A^2 \Delta B^2 \geq |\langle\psi|\widehat{A}'\widehat{B}'|\psi\rangle|^2 \tag{2}$$

Note that the right-hand side of this inequality can be interpreted as the squared modulus of the mean value $\overline{A'B'}$. Let us derive a lower bound for this quantity. To do so we decompose the operator $\widehat{A}'\widehat{B}'$ in its symmetric and skew-symmetric parts:

$$\widehat{A}'\widehat{B}' = \frac{1}{2}\left(\widehat{A}'\widehat{B}' + \widehat{B}'\widehat{A}'\right) + \frac{1}{2}\left(\widehat{A}'\widehat{B}' - \widehat{B}'\widehat{A}'\right)$$

The symmetric part is a Hermitian operator $\widehat{O}$ whose mean value must be purely real. The skew-symmetric part is exactly half of the commutator, so its mean value is $i\hbar/2$ by hypothesis. We conclude that

$$|\langle\psi|\widehat{A}'\widehat{B}'|\psi\rangle|^2 = \overline{O}^2 + \frac{\hbar^2}{4} \geq \frac{\hbar^2}{4} \tag{3}$$

Combining Eqs. (2) and (3), we have

$$\Delta A^2 \Delta B^2 \geq \frac{\hbar^2}{4}$$

so that

$$\Delta A \Delta B \geq \frac{\hbar}{2} \tag{4}$$

This is the famous Heisenberg inequality. We saw in Lecture 9 that the operators $\hat{x}$ and $\hat{p}_x$ satisfy $[\hat{x}, \hat{p}_x] = i\hbar$, so

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

The uncertainties in observation of p_x and x are always such that the product of the standard deviations is greater than $\hbar/2$.

2.3 Sufficient condition for compatibility

We will now prove that the condition $[\widehat{A}, \widehat{B}] = 0$ on the commutator of $\widehat{A}$ and $\widehat{B}$ is not only a necessary condition for compability between A and B, but also a sufficient condition. In order to keep the proof relatively simple, we will assume that the spectra of the operators is discrete. However, the results extend to the case of a continuous spectrum.

Let $|a\rangle$ be an eigenfunction of $\widehat{A}$ with eigenvalue a. We expand this eigenfunction on a basis of eigenfunctions of $\widehat{B}$:

$$|a\rangle = \sum_{n,(l)} c_{n,(l)} |b_n, (l)\rangle$$

We regroup all the terms associated with a given eigenvalue and write

$$|\beta_n\rangle = \sum_{(l)} c_{n,(l)} |b_n, (l)\rangle$$

so that

$$|a\rangle = \sum_n |\beta_n\rangle$$

In this expansion, all the terms correspond to a different eigenvalue of $\widehat{B}$. As a result, the $|\beta_n\rangle$ are all orthogonal to one another, and thus linearly independent. We will show that in addition, they are eigenfunctions of the operator $\widehat{A}$.

Consider the ket $|\chi_n\rangle = (\widehat{A} - a\hat{I})|\beta_n\rangle$. Note first that $|\chi_n\rangle$ is an eigenfunction of $\widehat{B}$. Indeed, $\hat{B}$ commutes with $\widehat{A} - a\hat{I}$ since $[\widehat{A}, \widehat{B}] = 0$ by hypothesis. Then

$$\widehat{B}(\widehat{A} - a\hat{I})|\beta_n\rangle = (\widehat{A} - a\hat{I})\widehat{B}|\beta_n\rangle = (\widehat{A} - a\hat{I})b_n|\beta_n\rangle = b_n|\chi_n\rangle$$

Since the eigenvalues b_n are all distinct, the $|\chi_n\rangle$ are linearly independent. And since $|a\rangle = \sum_n |\beta_n\rangle$,

$$\sum_n |\chi_n\rangle = \sum_n (\widehat{A} - a\hat{I})|\beta_n\rangle = (\widehat{A} - a\hat{I})\sum_n |\beta_n\rangle = (\widehat{A} - a\hat{I})|a\rangle = 0$$

we conclude that the $|\chi_n\rangle$ are all zero. In other words, the eigenfunctions $|\beta_n\rangle$ are also eigenfunctions of $\widehat{A}$. They are common to both $\widehat{A}$ and $\widehat{B}$.

Here is how we can see that we can construct a basis of common eigenfunctions of $\widehat{A}$ and $\widehat{B}$ in this manner. Take a general ket $|\psi\rangle$, and expand it on a basis of eigenfunctions $|a_m, (l)\rangle$ of $\widehat{A}$. We just showed that each $|a_m, (l)\rangle$ can itself be expanded in terms of eigenfunctions $|\beta_n\rangle$ of both $\widehat{A}$ and $\widehat{B}$. In this expansion, there may be terms with the same eigenvalue couple (a_m, b_n) that are not necessarily linearly independent. However, one may construct an orthonormal basis for the associated subspace through a Gram-Schmidt procedure. In the end, we have an orthonormal basis of eigenfunctions common to $\widehat{A}$ and $\widehat{B}$ and the corresponding observables are compatible.

The bottom line thus is that observables are compatible if and only if their associated operators commute.

3 Key role of the Hamiltonian

The Hamiltonian operator $\widehat{H}$ plays a key role in quantum mechanics since it determines the temporal evolution of the quantum system through the Schrödinger equation. In this section, we will explore a number of important properties of $\widehat{H}$.

3.1 Stationary states

We will work in $\mathbf{r}$ representation, and call $\phi_E(\mathbf{r}, t)$ the eigenfunctions of the operator $\widehat{H}$ with eigenvalue E:

$$\widehat{H}\phi_E(\mathbf{r}, t) = E\phi_E(\mathbf{r}, t) \tag{5}$$

Just like any other wave function, the time dependence of the ϕ_E is given by the Schrödinger equation

$$\widehat{H}\phi_E(\mathbf{r}, t) = i\hbar\frac{\partial \phi_E}{\partial t} \tag{6}$$

We can combine Eqs.(5) and (6) to write

$$i\hbar\frac{\partial \phi_E}{\partial t} = E\phi_E(\mathbf{r}, t) \tag{7}$$

We can solve this first order partial differential equation through separation of variables:

$$\phi_E(\mathbf{r}, t) = \chi_E(\mathbf{r})e^{-iEt/\hbar} \tag{8}$$

If χ_E is the state of the system at $t = 0$, then ϕ_E as given in Eq.(8) gives the state of the system for all $t > 0$ since it agrees with χ_E at $t = 0$ and it satisfies the Schrödinger equation.

Consider now an observable A that only depends on $\mathbf{r}$ and $\mathbf{p}$ in classical mechanics. Then time does not appear in the operator $\hat{A}$ either, and we can write the following equality for the mean value $\overline{A^n}$ for any $n \in \mathbb{N}^*$:

$$\overline{A^n} = \langle \phi_E(\mathbf{r}, t), \widehat{A}^n\phi_E(\mathbf{r}, t)\rangle = \langle \chi_E(\mathbf{r}), \widehat{A}^n\chi_E(\mathbf{r})\rangle$$

where equality holds because the factors $\exp(iEt/\hbar)$ cancel when one evaluates the inner product. Since χ_E does not depend on time, we see that $\overline{A^n}$ is time independent. And since this is true for all $n \in \mathbb{N}^*$, the statistical distribution of A is time independent.

We conclude that if at some point t_0 in time the system is in an eigenstate of the Hamiltonian, the system remains in that state for all time $t > t_0$, and the statistical distribution of all physical quantities is independent of time. Such a state is called a stationary state.

3.2 Conserved quantities

We just saw that when the system is in a stationary state, the statistical distributions of physical quantities are independent of time. We can also imagine situations in which the system is not in a stationary state, but a certain physical quantity has a statistical distribution that does not depend on time. In that case, we say that this physical quantity is a *conserved quantity*. This is the quantum mechanical equivalent of conserved quantities in classical mechanics.

Based on a key result we derived in Lecture 9, we will derive a sufficient condition for a quantity to be conserved in the quantum mechanical sense. Remember that for a physical quantity O and its associated operator $\widehat{O}$, we derived the following result on our way to Ehrenfest's equations:

$$\frac{d\overline{O}}{dt} = \frac{i}{\hbar}\overline{[\widehat{H},\widehat{O}]}$$

It is clear that if $\widehat{O}$ commutes with $\widehat{H}$, the mean value of O is time independent. One can then also say the same thing for any moment of O (since $\widehat{O^n}$ must then commute with $\widehat{H}$), so the statistical distribution of O is time independent. In conclusion, if an operator associated with a physical quantity commutes with the Hamiltonian, this physical quantity is conserved during the evolution of the system. In particular, if the system is initially in an eigenstate of the operator, any measurement will always obtain the same eigenvalue; in that case, the phrase conserved quantity has the same meaning as in the classical limit.

3.3 Time-Energy uncertainty relation

Assume that the eigenvalue spectrum of the Hamiltonian is discrete. There then is a basis of eigenfunctions $\chi_{n,(l)}(\mathbf{r})$ of the Hamiltonian with associated eigenvalue E_n. The general solution to the Schrödinger equation then us

$$\psi(\mathbf{r},t) = \sum_n c_{n,(l)}\chi_{n,(l)}(\mathbf{r})e^{-iE_nt/\hbar}$$

Note that the coefficients $c_{n,(l)}$ and the eigenfunctions χ are time-independent. The time dependence is given by the exponential factors only. Since the energy eigenvalue E_n is different in each term of the expansion, there will be time-dependent phase shifts between the different terms. When the probability amplitudes are evaluated, this will lead to time dependent interference phenomena.

Consider first a system with two energy levels E_1 and E_2:

$$\psi(\mathbf{r},t) = c_1\chi_1\exp(-iE_1t/\hbar) + c_2\chi_2\exp(-iE_2t/\hbar)$$

The probability density of presence of the system in a small interval d$\mathbf{r}$ is given by

$$|\psi|^2 = |c_1\chi_1|^2 + |c_2\chi_2|^2 + 2\Re\left\{c_1^*c_2\chi_1^*\chi_2\exp[-i(E_1-E_2)t/\hbar]\right\}$$

We see that the last term, the interference term, is the only one that depends on time, and the probability density varies with time according to an expression of the form

$$A + B\cos\left(\frac{(E_1-E_2)t}{\hbar} + \alpha\right)$$

It is therefore periodic, with period

$$\tau = \frac{2\pi\hbar}{|E_1-E_2|}$$

We see that the characteristic time of evolution is of the order $\hbar/\Delta E$, where $\Delta E = |E_1 - E_2|$ is the standard deviation of the distribution.

Consider another interesting example, in which there is an infinite countable number of energy levels that are evenly spaced: $E_n = E_0 + n\Delta E$, where ΔE is the spacing between energy levels. We then have

$$\psi(\mathbf{r},t) = \exp\left(-i\frac{E_0 t}{\hbar}\right)\left[\sum_{n=0}^{\infty} c_n \chi_n(\mathbf{r}) \exp\left(-\frac{in\Delta E t}{\hbar}\right)\right]$$

The quantity in square brackets is a Fourier series with period $\tau = 2\pi\hbar/\Delta E$. It is then clear that $|\psi|^2$ is also periodic with period $\tau = 2\pi\hbar/\Delta E$.

It turns out that even for the cases in which the spectrum is discrete but not evenly spaced, one can show that $\tau \sim \hbar/\Delta E$. Note that the evolution of the system is not periodic in that case, so τ may be seen as the characteristic time for the evolution of the system, and Δ is to be seen as the characteristic spacing between energy levels. The estimate $\tau \sim \hbar/\Delta E$ also holds for situations with a continuous spectrum.

The bottom line is that non-stationary systems have an energy distribution that is such that

$$\tau\Delta E \sim \hbar \tag{9}$$

Equation (9) is known as the time-energy uncertainty relation. Even though it looks quite similar to Heisenberg's inequalities, its meaning is slightly different in non-relativistic quantum mechanics, the framework we are working in. This makes sense since time in not an observable. However, we can also view the time-energy uncertainty relation as a sign that the de Broglie's relations

$$\mathbf{p} = \hbar\mathbf{k} \qquad E = \hbar\omega$$

are inherently consistent with the theory of relativity, which treats on an equal footing space and time through the four-vector $(\mathbf{r}, ct)$, and momentum and energy through the four-vector $(\mathbf{p}, E/c)$.

3.4 Invariance and conservation laws

Translations

Consider a system described in the $\mathbf{r}$ representation that is invariant under infinitesimal translations ϵ along the x-axis. This means that if $\Psi(x,y,z,t)$ is the original wave function that satisfies the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \widehat{H}\Psi$$

then the shifted wavefunction

$$\Psi_T(x,y,z,t) = \Psi(x-\epsilon,y,z,t) \tag{10}$$

also satisfies

$$i\hbar\frac{\partial\Psi_T}{\partial t} = \widehat{H}\Psi_T$$

Let us expand Eq.(10) to first order in ϵ:

$$\Psi_T(x,y,z,t) = \Psi(x,y,z,t) - \epsilon\frac{\partial\Psi}{\partial x} + O(\epsilon^2)$$

In other words, since $\widehat{p_x} = \hbar/i\partial/\partial x$, to first order in ϵ we can write

$$\Psi_T(x,y,z,t) = \left(\widehat{I} - \frac{i\epsilon}{\hbar}\widehat{p_x}\right)\Psi(x,y,z,t) \equiv \widehat{T}\Psi(x,y,z,t)$$

with

$$\widehat{T} = \widehat{I} - \frac{i\epsilon}{\hbar}\widehat{p_x}$$

Since $\widehat{T}$ does not depend on t, the Schrödinger equation for Ψ_T implies

$$\widehat{H}\Psi_T = i\hbar\frac{\partial\Psi_T}{\partial t} = i\hbar\frac{\partial\widehat{T}\Psi}{\partial t} = \widehat{T}\left(i\hbar\frac{\partial\Psi}{\partial t}\right) = \widehat{T}\widehat{H}\Psi$$

where the last equality holds because Ψ satisfies the Schrödinger equation. We conclude that

$$\widehat{H}\widehat{T}\Psi = \widehat{T}\widehat{H}\Psi$$

Since this is true for an arbitrary Ψ, we must have

$$[\widehat{H}, \widehat{T}] = 0$$

which implies

$$[\widehat{H}, \widehat{p_x}] = 0$$

According to Section 3.2, the last equality means that p_x is conserved. We recover here a well-known result of classical mechanics: invariance under translation in a given direction implies invariance of the conjugate momentum in that direction. This can be viewed as the quantum mechanical version of Noether's theorem for the momentum.

Rotations

Consider now the rotation with a small angle ϵ about the z axis:

$$\begin{cases} x' = x - \epsilon y \\ y' = y + \epsilon x \\ z' = z \end{cases}$$

Invariance under this rotation means that

$$\Psi_R(x, y, z) = \Psi(x + \epsilon y, y - \epsilon x, z)$$

also satisfies the Schrödinger equation. Now, proceeding as before, we have to first order in ϵ

$$\Psi_R(x, y, z) = \Psi(x, y, z) + \epsilon y \frac{\partial \Psi}{\partial x} - \epsilon x \frac{\partial \Psi}{\partial y} = \left[\widehat{I} - \frac{i\epsilon}{\hbar}(\hat{x}\widehat{p_y} - \hat{y}\widehat{p_x}) \right] \Psi \equiv \widehat{R}\Psi$$

In the second term of the operator $\widehat{R}$, the operator associated with the z-component of the angular momentum $\mathbf{r} \times \mathbf{p}$ appears; we call it $\widehat{L}_z$:

$$\widehat{R} = \widehat{I} - \frac{i\epsilon}{\hbar}\widehat{L}_z$$

Following the same steps as in the case of a translational symmetry, we conclude that invariance under this rotation implies that $[\widehat{H}, \widehat{L}_z] = 0$, and the z component of the angular momentum is conserved. This is another illustration of the quantum mechanical version of Noether's theorem.

Note that the operators $\widehat{L}_x$, $\widehat{L}_y$, and $\widehat{L}_z$ do not commute with one another: L_x, L_y, and L_z are therefore physical quantities that are not compatible.

3.5 Parity transformations

A parity transformation P corresponds to the flip in the sign of all three spatial coordinates: $P : (x, y, z) \mapsto (-x, -y, -z)$. In other words, it is a point reflection with respect to the origin. It is a transformation that transforms a right hand into a left hand.

Let us see what invariance under this transformation implies for the system.

We have $\Psi_T(x, y, z) = \widehat{P}\Psi(x, y, z) = \Psi(-x, -y, -z)$, where $\widehat{P}$ is called the parity operator. Clearly, $\widehat{P}^2 = \widehat{I}$ so $\widehat{P} = \widehat{P}^{-1}$. Furthermore, $\widehat{P}$ is Hermitian since for all χ and ψ,

$$\langle \chi, \widehat{P}\psi \rangle = \int \chi^*(\mathbf{r})\psi(-\mathbf{r})d\mathbf{r} = \int \chi^*(-\mathbf{r})\psi(\mathbf{r})d\mathbf{r} = \langle \widehat{P}\chi, \psi \rangle$$

where we have used the fact that the Jacobian of the change of variable $\mathbf{r} \to -\mathbf{r}$ is 1.

Since $\widehat{P}^2 = \widehat{I}$, the eigenvalues of $\widehat{P}$ are either 1 or -1. The eigenfunctions associated with the eigenvalue 1 are the even functions in the transformation $(x, y, z) \mapsto (-x, -y, -z)$. The eigenfunctions associated with the eigenvalue -1 are the odd functions in the transformation $(x, y, z) \mapsto (-x, -y, -z)$.

Following the two previous sections, the operator $\widehat{P}$ commutes with $\widehat{H}$ if the system is invariant under the parity transformation. In that case, if a wave function is initially even or odd, it remains even or odd throughout the time evolution.

A simple example of this corresponds to the situation studied in Problem 3 of Homework 5. The potential well satisfies $U(x) = U(-x)$, so the system is invariant under the parity transformation. That means that $\widehat{P}$ and $\widehat{H}$ commute, and as a result have a common basis of eigenfunctions. These eigenfunctions have either odd or even parity, as we found in that problem.