2.1: Basic Relations

As was discussed at the end of Chapter 1, in several cases (in particular, at strong confinement within the $[y, z]$ plane), the general (3D) Schrödinger equation may be reduced to its 1D version, similar to Eq. (1.92):

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x,t)\Psi(x,t) \tag{2.1.1}$$

It is important, however, to remember that according to the discussion in Sec, $1.8, U(x,t)$ in this equation is generally effective potential energy, which may include the energy of the lateral motion, while $\Psi(x,t)$ may be just one factor in the complete wavefunction $\Psi(x,t)\chi(y,z)$. If the transverse factor $\chi(y,z)$ is normalized to 1 , then the integration of Eq. (1.22a) over the 3D space within a segment $[x_1, x_2]$ gives the following probability to find the particle on this segment:

$$W(t) \equiv \int_{x_1}^{x_2} \Psi(x,t)\Psi^*(x,t)dx \tag{2.1.2}$$

If the particle under analysis is definitely somewhere inside the system, the normalization of its 1D wavefunction $\Psi(x,t)$ is provided by extending integral (2) to the whole axis x :

Normalization

$$\int_{-\infty}^{+\infty} w(x,t)dx = 1, \text{ where } w(x,t) \equiv \Psi(x,t)\Psi^*(x,t). \tag{2.1.3}$$

A similar integration of Eq. (1.23) shows that the expectation value of any observable depending only on the coordinate x (and possibly time), may be expressed as

$$\langle A\rangle(t) = \int_{-\infty}^{+\infty} \Psi^*(x,t)\hat{A}\Psi(x,t)dx. \tag{2.1.4}$$

It is also useful to introduce the notion of the probability current along the x-axis (a scalar):

$$I(x,t) \equiv \int j_x dydz = \frac{\hbar}{m}\operatorname{Im}\left(\Psi^* \frac{\partial}{\partial x}\Psi\right) = \frac{\hbar}{m}|\Psi(x,t)|^2 \frac{\partial \varphi}{\partial x}, \tag{2.1.5}$$

where j_x is the x-component of the current density vector $\mathbf{j}(\mathbf{r},t)$. Then the continuity equation (1.48) for any segment $[x_1, x_2]$ takes the form

$$\frac{dW}{dt} + I(x_2) - I(x_1) = 0 \tag{2.1.6}$$

The above formulas are sufficient for analysis of 1D problems of wave mechanics, but before proceeding to particular cases, let me deliver on my earlier promise to prove that Heisenberg's uncertainty relation (1.35) is indeed valid for any wavefunction $\Psi(x,t)$. For that, let us consider the following positive (or at least non-negative) integral

$$J(\lambda) \equiv \int_{-\infty}^{+\infty} \left| x\Psi + \lambda \frac{\partial \Psi}{\partial x}\right|^2 dx \geq 0, \tag{2.1.7}$$

where λ is an arbitrary real constant, and assume that at $x \to \pm\infty$ the wavefunction vanishes, together with its first derivative - as we will see below, a very common case. Then the left-hand side of Eq. (7) may be recast as

$$\begin{aligned} J(\lambda) &\equiv \int_{-\infty}^{+\infty} \left| x\Psi + \lambda \frac{\partial \Psi}{\partial x}\right|^2 dx = \int_{-\infty}^{+\infty} \left(x\Psi + \lambda\frac{\partial \Psi}{\partial x}\right)\left(x\Psi + \lambda\frac{\partial \Psi}{\partial x}\right)^* dx \\ &= \int_{-\infty}^{+\infty} x^2\Psi\Psi^* dx + \lambda\int_{-\infty}^{+\infty} x\left(\Psi\frac{\partial \Psi *}{\partial x} + \frac{\partial \Psi}{\partial x}\Psi^*\right)dx + \lambda^2\int_{-\infty}^{+\infty} \frac{\partial \Psi}{\partial x}\frac{\partial \Psi^*}{\partial x}dx. \end{aligned}$$

According to Eq. (4), the first term in the last form of Eq. (8) is just $\langle x^2\rangle$, while the second and the third integrals may be worked out by parts:

$$\int_{-\infty}^{+\infty} x\left(\Psi \frac{\partial \Psi^*}{\partial x}+\frac{\partial \Psi}{\partial x} \Psi^*\right) d x \equiv \int_{-\infty}^{+\infty} x \frac{\partial}{\partial x}\left(\Psi \Psi^*\right) d x=\int_{x=-\infty}^{x=+\infty} x d\left(\Psi \Psi^*\right)=\Psi \Psi^* x \mid \begin{array}{l} x=+\infty \\ x=-\infty \end{array}-\int_{-\infty}^{+\infty} \Psi \Psi^* d x$$

$$=-1,$$

$$\int_{-\infty}^{+\infty} \frac{\partial \Psi}{\partial x} \frac{\partial \Psi^*}{\partial x} d x=\int_{x=-\infty}^{x=+\infty} \frac{\partial \Psi}{\partial x} d \Psi^*=\frac{\partial \Psi}{\partial x} \Psi^* \mid \begin{array}{l} x=+\infty \\ x=-\infty \end{array}-\int_{-\infty}^{+\infty} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} d x=\frac{1}{\hbar^2} \int_{-\infty}^{+\infty} \Psi^* \hat{p}_x^2 \Psi d x=\frac{\left\langle p_x^2\right\rangle}{\hbar^2}$$

As a result, Eq. (7) takes the following form:

$$J(\lambda)=\left\langle x^2\right\rangle-\lambda+\lambda^2 \frac{\left\langle p_x^2\right\rangle}{\hbar^2} \geq 0, \text{ i.e. } \lambda^2+a \lambda+b \geq 0, \quad \text{with } a \equiv-\frac{\hbar^2}{\left\langle p_x^2\right\rangle}, b \equiv \frac{\hbar^2\left\langle x^2\right\rangle}{\left\langle p_x^2\right\rangle}. \tag{2.1.8}$$

This inequality should be valid for any real λ, so that the corresponding quadratic equation, $\lambda^2+a \lambda+b=0$, can have either one (degenerate) real root - or no real roots at all. This is only possible if its determinant, $\operatorname{Det}=a^2-4 b$, is non-positive, leading to the following requirement:

$$\left\langle x^2\right\rangle\left\langle p_x^2\right\rangle \geq \frac{\hbar^2}{4}. \tag{2.1.9}$$

In particular, if $\langle x\rangle=0$ and $\left\langle p_x\right\rangle=0$,[1] then according to Eq. (1.33), Eq. (12) takes the form

$$\text{Heisenberg's uncertainty relation} \qquad \left\langle\tilde{x}^2\right\rangle\left\langle\tilde{p}_x^2\right\rangle \geq \frac{\hbar^2}{4}, \tag{2.13}$$

which, according to the definition (1.34) of the r.m.s. uncertainties, is equivalent to Eq. (1.35).

Now let us notice that the Heisenberg's uncertainty relation looks very similar to the commutation relation between the corresponding operators:

$$\left[\hat{x}, \hat{p}_x\right] \Psi \equiv\left(\hat{x} \hat{p}_x-\hat{p}_x \hat{x}\right) \Psi=x\left(-i \hbar \frac{\partial \Psi}{\partial x}\right)-\left(-i \hbar \frac{\partial}{\partial x}\right)(x \Psi)=i \hbar \Psi. \tag{2.1.10}$$

Since this relation is valid for any wavefunction $\Psi(x, t)$, it may be represented as an operator equality:

$$\left[\hat{x}, \hat{p}_x\right]=i \hbar \neq 0. \tag{2.1.11}$$

In Sec. 4.5 we will see that the relation between Eqs. (13) and (14) is just a particular case of a general relation between the expectation values of non-commuting operators, and their commutators.

[1] Eq. (13) may be proved even if $\langle x\rangle$ and $\left\langle p_x\right\rangle$ are not equal to zero, by making the following replacements: $x \rightarrow x-\langle x\rangle$ and $\partial / \partial x \rightarrow \partial / \partial x+i\langle p\rangle / \hbar$ in Eq. (7), and then repeating all the calculations - which in this case become somewhat bulky. In Chapter 4, equipped with the bra-ket formalism, we will derive a more general uncertainty relation, which includes the Heisenberg's relation (13) as a particular case, in a more efficient way.