Chapter 1
Recollections from Elementary Quantum Physics

Abstract We recall the prerequisites that we assume the reader to be familiar with, namely the Schrödinger equation in its time dependent and time independent form, the uncertainty relations, and the basic properties of angular momentum.

Introductory courses on quantum physics discuss the one-dimensional Schrödinger equation for the *wave function* $\Psi(x,t)$ of a particle of mass M moving in a potential V

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2M}\frac{\partial^2\Psi}{\partial x^2} + V\Psi. \tag{1.1}$$

Therein $\hbar = h/2\pi$ is the reduced Planck constant. The function Ψ is understood as a probability amplitude whose absolute square $|\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t)$ gives the *probability density* for finding the particle at time t at position x. This probability density is insensitive to a *phase factor* $\mathrm{e}^{\mathrm{i}\varphi}$. With the *Hamilton operator*

$$\mathrm{H} = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial x^2} + V, \tag{1.2}$$

the Schrödinger equation reads

$$\dot{\Psi} = -\frac{\mathrm{i}}{\hbar}\mathrm{H}\Psi. \tag{1.3}$$

The dot denotes the time derivative.

In this text, we print operators and matrices in nonitalic type, like H, $\mathbf{p}$, or $\boldsymbol{\sigma}$, just to remind the reader that a simple letter may represent a mathematical object more complicated than a number or a function. Ordinary vectors in three-dimensional space are written in bold italic type, like $\boldsymbol{x}$ or $\boldsymbol{B}$.

The time dependent Schrödinger equation reminds us of the law of energy conservation $E = p^2/2M + V$ if we associate the operator $\mathrm{i}\hbar\partial/\partial t$ with energy E and the operator $(\hbar/\mathrm{i})\partial/\partial x$ with momentum p. Take as an example the plane wave $\Psi(x,t) = \Psi_0\mathrm{e}^{\mathrm{i}(kx-\omega t)}$ of a photon propagating in the x-direction. The energy operation $\mathrm{i}\hbar\partial\Psi/\partial t = \hbar\omega\Psi$ then relates energy to frequency, $E = \hbar\omega$, and the momentum operation $(\hbar/\mathrm{i})\partial\Psi/\partial x = \hbar k\Psi$ relates momentum to wave number, $p = \hbar k$.

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The probability amplitude $\Psi(x,t)$ for finding the particle at time t at position x and the amplitude $\Phi(p,E)$ for finding it with energy E and momentum p turn out to be *Fourier transforms* of each other. Pairs of Fourier transforms have widths that are reciprocal to each other. If the width Δx in position is large, the width Δp in momentum is small, and vice versa, and the same for the widths Δt and ΔE. The *conjugate observables* p and x or E and t obey the *uncertainty relations*

$$\Delta p \Delta x \geq \frac{1}{2}\hbar, \qquad \Delta E \Delta t \geq \frac{1}{2}\hbar. \tag{1.4}$$

The exact meaning of Δx, etc. will be defined in Sect. 3.4.

For *stationary*, that is, time independent potentials $V(x)$, the Hamilton operator (1.2) acts only on the position variable x. The solution of the Schrödinger equation then is *separable* in x and t,

$$\Psi(x,t) = \psi(x)\mathrm{e}^{-\mathrm{i}Et/\hbar}. \tag{1.5}$$

The probability density (in units of m^{-1}) for finding a particle at position x then is independent of time $|\Psi(x,t)|^2 = |\psi(x)|^2$. The amplitude $\psi(x)$ is a solution of the *time independent* Schrödinger equation

$$-\frac{\hbar^2}{2M}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x). \tag{1.6}$$

In operator notation, this reads

$$\mathrm{H}\psi = E\psi. \tag{1.7}$$

For particles trapped in a potential well $V(x)$, the requirement that total probability is *normalizable* to

$$\int_{-\infty}^{+\infty} \left|\psi(x)\right|^2 \mathrm{d}x = 1 \tag{1.8}$$

leads to the *quantization of energy* E such that only a discrete set of values E_n, with the corresponding wave functions $\psi_n(x)$, $n = 1, 2, 3, \ldots$, is allowed. n is called the *main quantum number*.

The mean value derived from repeated measurements of a physical quantity or *observable* A is given by its *expectation value*

$$\left\langle A(t)\right\rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) A \Psi(x,t)\,\mathrm{d}x. \tag{1.9}$$

For a stationary state Eq. (1.5), the expectation value $\langle A\rangle$ does not depend on time and is insensitive to any phase factor $\mathrm{e}^{\mathrm{i}\varphi}$. For example, the mean position $\langle x\rangle$ of a matter wave is given by the weighted average

$$\langle x\rangle = \int_{-\infty}^{+\infty} x\left|\psi(x)\right|^2 \mathrm{d}x. \tag{1.10}$$

Sometimes the Hamiltonian H can be divided into two parts $\mathrm{H} = \mathrm{H}_1(\boldsymbol{x}) + \mathrm{H}_2(\boldsymbol{y})$, one depending on one set of (not necessarily spatial) variables $\boldsymbol{x}$, the other on a disjoint set of variables $\boldsymbol{y}$. Then, as shown in standard textbooks, the solution of the Schrödinger equation is separable in $\boldsymbol{x}$ and $\boldsymbol{y}$ as $\psi(\boldsymbol{x}, \boldsymbol{y}) = \psi_1(\boldsymbol{x})\psi_2(\boldsymbol{y})$. As in Eq. (1.5), we must attach a phase factor to obtain the time dependent solution

$$\Psi(\boldsymbol{x}, \boldsymbol{y}, t) = \psi_1(x)\psi_2(\boldsymbol{y})\mathrm{e}^{-\mathrm{i}Et/\hbar}. \tag{1.11}$$

The probability densities for the joint occurrence of variable $\boldsymbol{x}$ and variable $\boldsymbol{y}$ then multiply to

$$\left|\Psi(\boldsymbol{x}, \boldsymbol{y}, t)\right|^2 = \left|\psi_1(\boldsymbol{x})\right|^2 \left|\psi_2(\boldsymbol{y})\right|^2. \tag{1.12}$$

This is consistent with classical probability theory, where probabilities multiply for independent events. The probability that two dice both show 5 is $\frac{1}{6} \times \frac{1}{6} = \frac{1}{36}$.

If, on the other hand, the quantum system can evolve along two mutually exclusive paths ψ_1 or ψ_2, as is the case in the famous double-slit experiments, then the two probability amplitudes add *coherently*, and the total probability is

$$|\Psi|^2 = |\psi_1 + \psi_2|^2 = |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2| \sin\delta, \tag{1.13}$$

with phase angle δ. Only if phase coherence between the partial waves ψ_1 and ψ_2 is lost, does the total probability equal the classical result

$$|\Psi|^2 = |\psi_1|^2 + |\psi_2|^2, \tag{1.14}$$

with probabilities adding for mutually exclusive events. The probability that a die shows either 5 or 3 is $\frac{1}{6} + \frac{1}{6} = \frac{1}{3}$.

Figure 1.1 shows the setup and result of a double-slit experiment with a beam of slow neutrons. What we see is the self-interference of the probability amplitudes ψ_1 and ψ_2 of single neutrons. The conditions for the appearance of quantum interference will be discussed in Sect. 6.6.

For most students the Schrödinger equation is no more difficult than the many other differential equations encountered in mechanics, electrodynamics, or transport theory. Therefore, students usually have fewer problems with the ordinary Schrödinger equation than with a presentation of quantum mechanics in the form of matrix mechanics. In everyday scientific life, however, spectroscopic problems that require matrix diagonalization are more frequent than problems like particle waves encountering step potentials and other scattering problems. Furthermore, as we shall see in Sect. 19.1.2, the Schrödinger equation can always equally well be expressed as a matrix equation. Therefore, matrix mechanics is the main topic of the present tutorial. Instead of starting with the Schrödinger equation, we could have started with the Heisenberg equation of motion (discovered a few weeks before the Schrödinger equation) because both are equivalent. We postpone the introduction of Heisenberg's equation to Chap. 10 because students are less familiar with this approach.

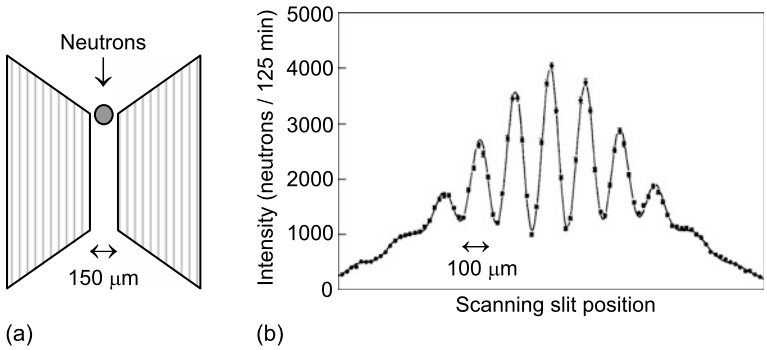

Fig. 1.1 (**a**) Double-slit experiment with neutrons: The monochromatic beam (*along the arrow*), of de Broglie wave length $\lambda = 2$ nm, $\Delta\lambda/\lambda = 8$ %, meets two slits, formed by a beryllium wire (*shaded circle*) and two neutron absorbing glass edges (*vertical hatching*), installed on an optical bench of 10 m length with 20 μm wide entrance and exit slits. (**b**) The measured neutron self-interference pattern follows theoretical expectation. From Zeilinger et al. (1988)

To begin we further assume acquaintance with some basic statements of quantum physics that are both revolutionary and demanding, and our hope is that the reader of this text will learn how to live and work with them. The first statement is: To any physical observable A corresponds an operator A. The measurement of the observable A leaves the system under study in one of the *eigenstates* or *eigenfunctions* ψ_n of this operator such that

$$\mathrm{A}\psi_n = a_n\psi_n. \tag{1.15}$$

The possible outcomes of the measurement are limited to the *eigenvalues* a_n. Which of these eigenfunctions and eigenvalues is singled out by the measurement is uncertain until the measurement is actually done.

If we regard the ordered list ψ_n as elements of a vector space, called the Hilbert space, the operation A just stretches an eigenvector ψ_n of this space by a factor a_n. The best-known example of an eigenvalue equation of this type is the time independent Schrödinger equation

$$\mathrm{H}\psi_n = E_n\psi_n. \tag{1.16}$$

H is the operator for the observable energy E, ψ_n are the eigenfunctions of energy, and E_n are the corresponding eigenvalues. In this text, we shall only treat the simplest case where the spectrum of the E_n is *discrete* and enumerable, as are atomic energy spectra, and in most cases limit the number of energy levels to two.

Another basic statement is derived in Sect. 3.4: Two physical quantities, described by operators A and B, can assume well defined values a_n and b_n, simultaneously measurable with arbitrarily high precision and unhampered by any uncertainty relation, if and only if they share a common set of eigenfunctions ψ_n, with

$$\mathrm{A}\psi_n = a_n\psi_n, \qquad \mathrm{B}\psi_n = b_n\psi_n. \tag{1.17}$$

An important operator is that of the *angular momentum* $\mathbf{J}$, which we shall derive from first principles in Chap. 16. Let us beforehand recapitulate the following properties of $\mathbf{J}$, as known from introductory quantum physics. The components J_x, J_y, and J_z of the angular momentum operator $\mathbf{J}$ cannot be measured simultaneously to arbitrary precision. Only the square magnitude $\mathbf{J}^2$ of the angular momentum and its component J_z along an arbitrary axis z are well defined and can be measured simultaneously without uncertainty. This means that the phase of $\mathbf{J}$ about this axis z remains uncertain. The operators of the two observables $\mathbf{J}^2$ and J_z then must have simultaneous eigenfunctions that we call ψ_{jm}, which obey

$$\mathbf{J}^2\psi_{jm} = j(j+1)\hbar^2\psi_{jm}, \tag{1.18a}$$

$$\mathrm{J}_z\psi_{jm} = m\hbar\psi_{jm}, \tag{1.18b}$$

with eigenvalues $j(j+1)\hbar^2$ and $m\hbar$, respectively.

Angular momentum is quantized, with possible *angular momentum quantum numbers* $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$. For a given value of j, the *magnetic quantum number* m can take on only the $2j+1$ different values $m = -j, -j+1, \ldots, j$.

For $j = \frac{1}{2}$ we have $m = \pm\frac{1}{2}$ and

$$\mathbf{J}^2\psi_{\frac{1}{2},\pm\frac{1}{2}} = \frac{3}{4}\hbar^2\psi_{\frac{1}{2},\pm\frac{1}{2}}, \tag{1.19a}$$

$$\mathrm{J}_z\psi_{\frac{1}{2},\pm\frac{1}{2}} = \pm\frac{1}{2}\hbar\psi_{\frac{1}{2},\pm\frac{1}{2}}. \tag{1.19b}$$

If we arrange the $2j+1$ eigenfunctions of the angular momentum ψ_{jm} into one column

$$\psi_j = \begin{pmatrix} \psi_{j,j} \\ \psi_{j,j-1} \\ \vdots \\ \psi_{j,-j} \end{pmatrix}, \tag{1.20}$$

we shall print this column vector ψ_j in nonitalic type, as we did for the operators. The corresponding row vector is $\psi_j^\dagger = (\psi_{j,j}^*, \psi_{j,j-1}^*, \ldots, \psi_{j,-j}^*)$, where the dagger signifies the *conjugate transpose* $\psi^\dagger = \psi^{*\mathrm{T}}$ of a complex vector (or matrix).

The components J_x and J_y of the angular momentum operator $\mathbf{J}$ do not have simultaneous eigenfunctions with $\mathbf{J}^2$ and J_z. If we form the linear combinations

$$\mathrm{J}_+ = \mathrm{J}_x + \mathrm{i}\mathrm{J}_y, \qquad \mathrm{J}_- = \mathrm{J}_x - \mathrm{i}\mathrm{J}_y, \tag{1.21}$$

these operators are found to act on the angular momentum state ψ_{jm} as

$$\mathrm{J}_+\psi_{jm} = \hbar\sqrt{j(j+1) - m(m+1)}\,\psi_{j,m+1}, \tag{1.22a}$$

$$\mathrm{J}_-\psi_{jm} = \hbar\sqrt{j(j+1) - m(m-1)}\,\psi_{j,m-1}, \tag{1.22b}$$

with $J_+\psi_{j,+j} = 0$ and $J_-\psi_{j,-j} = 0$. The J_+ and J_- are the *raising* and *lowering operators*, respectively. For $j = \frac{1}{2}$ we have $J_+\psi_{\frac{1}{2},-\frac{1}{2}} = \hbar\psi_{\frac{1}{2},+\frac{1}{2}}$ and $J_-\psi_{\frac{1}{2},+\frac{1}{2}} = \hbar\psi_{\frac{1}{2},-\frac{1}{2}}$.

Angular momentum may be composed of the *orbital* angular momentum $\mathbf{L}$ and of *spin* angular momentum $\mathbf{S}$, which can be added to the *total* angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$. The orbital angular momentum quantum number l can only have integer values, spin quantum number s can have either integer or half-integer values. The *triangle rule* of vector addition tells us that the (integer or half-integer) angular momentum quantum number j has the allowed range

$$|l - s| \leq j \leq l + s. \tag{1.23}$$

The total angular momentum quantum number is

$$m = m_l + m_s, \tag{1.24}$$

going in unit steps from $m = -j$ to $m = j$. For example, two angular momenta with $l = 1$ and $s = \frac{1}{2}$ can be added to $j = \frac{1}{2}$ or $j = \frac{3}{2}$. For $l = 0$, $j = s$ we have $m = m_s$, and for $s = 0$, $j = l$ we have $m = m_l$. For the sake of simplicity, in these two special cases we shall always write m for the respective magnetic quantum numbers m_s or m_l.

References

Zeilinger, A., Gähler, R., Shull, C.G., Treimer, W., Mampe, W.: Single- and double-slit diffraction of neutrons. Rev. Mod. Phys. **60**, 1067–1073 (1988)

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