Chapter 4
The Schrödinger Realization of Quantum Mechanics

The realization of the basic principles of quantum mechanics by means of position wave functions is presented in Sect. 4.1. This is where the time-independent Schrödinger equation is obtained, and where the spatial dimension in quantum problems appears explicitly.

The harmonic oscillator problem is solved again in Sect. 4.2. The reader will thus be able to contrast two realizations of quantum mechanics by comparing the results obtained here with those presented in Sect. 3.3.

Solutions to the Schrödinger equation in the absence of forces are discussed in Sect. 4.3. Such solutions present normalization problems which are solved by taking into consideration the limiting case of particles moving either in a large, infinitely deep square well potential, or along a circumference with a large radius (Sect. 4.4.1). These solutions are applied to some situations that are interesting both conceptually and in practical applications: the step potential (Sect. 4.5.1) and the square barrier (Sect. 4.5.2), which are schematic versions of scattering experiments. The free-particle solutions are also applied to the bound-state problem of the finite square well (Sect. 4.4.2), to the periodic potential (Sect. 4.6†) and to a practical application, the tunneling microscope (Sect. 4.5.3).

4.1 Time-Independent Schrödinger Equation

In the formulation of quantum mechanics presented in this chapter, the state vector is a complex function of the coordinate, $\Psi = \Psi(x)$. This type of state vector is usually known as a wave function. The sum of two wave functions is another wave function

$$\Psi(x) = \alpha_B \Psi_B(x) + \alpha_C \Psi_C(x). \tag{4.1}$$

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The scalar product is defined as

$$\langle \Psi_B | \Psi_C \rangle = \int_{-\infty}^{\infty} \Psi_B^* \Psi_C \, \mathrm{d}x. \tag{4.2}$$

As a consequence of this choice of $\Psi(x)$, the coordinate operator is simply the coordinate itself

$$\hat{x} = x. \tag{4.3}$$

A realization of the algebra (2.15) is given by the assignment[1]

$$\hat{p} = -\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}x}, \tag{4.4}$$

since for an arbitrary function $f(x)$,

$$[x, \hat{p}] f = -\mathrm{i}\hbar x \frac{\mathrm{d}f}{\mathrm{d}x} + \mathrm{i}\hbar \frac{\mathrm{d}(xf)}{\mathrm{d}x} = \mathrm{i}\hbar f. \tag{4.5}$$

It is simple to verify that the operator x is Hermitian, according to the definition (2.53). This is also true for the momentum operator, since

$$\int_{-\infty}^{\infty} \Phi^* \hat{p} \Psi \mathrm{d}x = -\mathrm{i}\hbar \Phi^* \Psi|_{-\infty}^{\infty} + \mathrm{i}\hbar \int_{-\infty}^{\infty} \Psi \frac{\mathrm{d}}{\mathrm{d}x} \Phi^* = \left(\int_{-\infty}^{\infty} \Psi^* \hat{p} \Phi \mathrm{d}x \right)^*, \tag{4.6}$$

where we have assumed $\Psi(\pm\infty) = 0$, as is the case for bound systems. The eigenfunctions of the momentum operator are discussed in Sect. 4.3.

A translation of the state vector by the amount a can be performed by means of the unitary operator

$$\mathcal{U}(a) = \exp\left(\frac{\mathrm{i}}{\hbar} a \hat{p} \right), \tag{4.7}$$

since

$$\mathcal{U}(a)\Psi(x) = \sum_n \frac{a^n}{n!} \frac{\mathrm{d}^n \Psi}{\mathrm{d}x^n} = \Psi(x + a). \tag{4.8}$$

An observable is translated as

$$\mathcal{U} \hat{Q}(x) \mathcal{U}^+ = \hat{Q}(x + a). \tag{4.9}$$

A finite translation may be generated by a series of infinitesimal steps

$$\mathcal{U}(\delta a) = 1 + \frac{\mathrm{i}}{\hbar} \delta a \, \hat{p}, \tag{4.10}$$

and $\hat{p}$ is referred to as the generator of infinitesimal translations.

[1]Although any function of x may be added to (4.4) and still satisfy (2.15), such a term should be dropped because free space is homogeneous.

The replacement of the operators (4.3) and (4.4) in the classical expression of any physical observable $Q(x, p)$ yields the corresponding quantum mechanical operator $\hat{Q} = Q(x, \hat{p})$ in a differential form. Given any complete set of orthonormal wave functions $\varphi_i(x)$, the matrix elements associated with the operator $\hat{Q}$ are constructed as in (2.10). This construction provides the link between the Heisenberg and the Schrödinger realizations of quantum mechanics.

The conservation law associated with translational symmetry is expressed by the commutation $[\hat{H}, \hat{p}] = 0$. This is the second symmetry that we have come across in the present text.

The Hamiltonian (2.16) yields the eigenvalue equation

$$-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2\varphi_i}{\mathrm{d}x^2} + V(x)\varphi_i = E_i\varphi_i, \tag{4.11}$$

which is called the time-independent Schrödinger equation.

4.1.1 *Probabilistic Interpretation of Wave Functions*

Information may be extracted from the wave function through the probability density (2.71) [31]

$$\rho(x) = |\Psi(x)|^2. \tag{4.12}$$

The probability of finding the particle in the interval $L_1 \leq x \leq L_2$ is given by the integral

$$\int_{L_1}^{L_2} |\Psi(x)|^2 \mathrm{d}x. \tag{4.13}$$

In particular, the probability of finding the particle anywhere must equal 1:

$$1 = \langle\Psi|\Psi\rangle, \tag{4.14}$$

which implies that the wave function should be normalized.

We now discuss how this probability changes with time t. We therefore allow for a time dependence of the wave function[2] $[\Psi = \Psi(x, t)]$:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{L_1}^{L_2} |\Psi(x,t)|^2 \mathrm{d}x &= \int_{L_1}^{L_2} \left(\dot{\Psi}^*\Psi + \Psi^*\dot{\Psi}\right)\mathrm{d}x \\ &= \frac{\mathrm{i}}{\hbar}\int_{L_1}^{L_2} \left[\left(\mathrm{i}\hbar\dot{\Psi}\right)^*\Psi - \Psi^*\left(\mathrm{i}\hbar\dot{\Psi}\right)\right]\mathrm{d}x. \end{aligned} \tag{4.15}$$

[2]The time dependence of the wave function is discussed in Chap. 9. We anticipate the result here because the notion of probability current is needed in the next few sections.

We may replace $\mathrm{i}\hbar\dot{\Psi}$ with $\hat{H}\Psi$, according to the time-dependent Schrödinger equation (9.5). We are left with only the kinetic energy contribution, since the terms proportional to the potential cancel inside (4.15):

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{L_1}^{L_2}|\Psi(x,t)|^2\mathrm{d}x = -\frac{\mathrm{i}\hbar}{2M}\int_{L_1}^{L_2}\left(\frac{\mathrm{d}^2\Psi^*}{\mathrm{d}x^2}\Psi - \Psi^*\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2}\right)\mathrm{d}x$$
$$= \frac{\mathrm{i}\hbar}{2M}\int_{L_1}^{L_2}\frac{\mathrm{d}}{\mathrm{d}x}\left(-\frac{\mathrm{d}\Psi^*}{\mathrm{d}x}\Psi + \Psi^*\frac{\mathrm{d}\Psi}{\mathrm{d}x}\right). \tag{4.16}$$

We obtain the equation

$$\frac{\partial\rho}{\partial t} + \frac{\partial j}{\partial x} = 0, \tag{4.17}$$

where we have defined the probability current

$$j(x,t) \equiv -\frac{\mathrm{i}\hbar}{2M}\left(-\frac{\partial\Psi^*}{\partial x}\Psi + \Psi^*\frac{\partial\Psi}{\partial x}\right). \tag{4.18}$$

Equation (4.17) is a continuity equation, similar to the one used in hydrodynamics to express conservation of mass. Imagine a long prism along the x-axis, bound by two squares of area $\mathcal{A}$ at $x = L_1$ and $x = L_2$, respectively. The variation of the probability of finding the particle inside the prism, i.e.

$$-\frac{\partial}{\partial t}\int_{L_1}^{L_2}\rho\,\mathrm{d}x,$$

is equal to the difference between the fluxes leaving and entering the prism, viz. $\mathcal{A}[j(L_2) - j(L_1)]$ (see Fig. 4.1).

The probability density and the probability current give spatial dimensions to the Schrödinger realization of quantum mechanics. These spatial features are especially useful in chemistry, where bulges of electron distribution in atoms are associated with increases in the chemical affinities of elements (Fig. 5.2).

The expression for the probability current underscores the need to use complex state vectors in quantum mechanics, since the current vanishes for real wave functions.

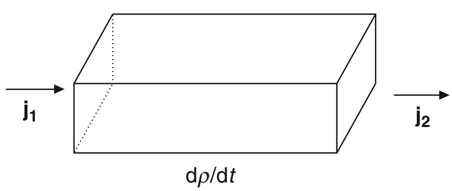

Fig. 4.1 Conservation of probability density. The rate of change within a certain interval is given by the flux differences at the boundaries of the interval

Here we may continue the list of misconceptions that prevail in quantum mechanics [19]:

- "The probability current $j(x)$ is related to the speed of that part of the particle which is located at the position x." This statement gives the false impression that, although the particle as a whole has neither a definite position nor a definite momentum, it is made up of parts that do. In fact, particles are not made up of parts.
- "For any energy eigenstate, the probability density must have the same symmetry as the Hamiltonian." This statement is correct in the case of inversion symmetry, for even states of a parity-invariant Hamiltonian (see Sect. 4.2). It is not correct for odd states. It is also generally false for a central potential, since only $l = 0$ states have probability densities with a spherical shape (Fig. 5.2).
- "A quantum state $\Psi(x)$ is completely specified by its associated probability density $|\Psi(x)|^2$." The probability densities, being real numbers, cannot give information about all the properties of the state, such as, for example, those related to momentum.
- "The wave function is dimensionless." It has the dimensions $[\text{length}]^{-dN/2}$, where N is the number of particles and d is the dimension of the space.
- "The wave function $\Psi(x)$ is a function of regular three-dimensional space." This is true only for one-particle systems. For two-particle systems, the wave function $\Psi(x_1, x_2)$ exists in six-dimensional, configuration space.
- "The wave function is similar to other waves appearing in classical physics." Unlike electromagnetic or sound waves, the wave function is an abstract entity. In particular, it does not interact with particles.

Both the probability density and the probability current are defined at each point in space. Other quantum predictions require integration over the whole space. For instance, the expectation value of an operator $\hat{Q}$ is

$$\langle\Psi|Q|\Psi\rangle \equiv \int_{-\infty}^{\infty} \Psi(x,t)^* \hat{Q}\Psi(x,t)\mathrm{d}x. \tag{4.19}$$

For an operator depending only on the coordinate x, this definition is a direct consequence of Born's probability density (4.12). However, for a differential operator such as $\hat{p}$, the alternative $\int \Psi(\hat{Q}\Psi)^*\mathrm{d}x$ is also possible. Nevertheless, the two definitions are identical for physical (Hermitian) operators.

4.2 The Harmonic Oscillator Revisited

The Schrödinger equation (4.11) corresponding to the harmonic oscillator Hamiltonian (3.25) reads

$$-\frac{\hbar^2}{2M}\frac{\mathrm{d}^2\varphi_n(x)}{\mathrm{d}x^2}+\frac{M\omega^2}{2}x^2\varphi_n(x)=E_n\varphi_n(x). \tag{4.20}$$

4.2.1 Solution of the Schrödinger Equation

It is always useful to rewrite any equation in terms of dimensionless coordinates. Not only does one get rid of unnecessarily cumbersome constants, but the solution may apply just as well to cases other than the one being considered. Therefore, in the present problem, the coordinate x and the energy E are divided by the value of the characteristic length and energy (3.28), namely

$$u=x/x_{\mathrm{c}}, \qquad e=E/\hbar\omega. \tag{4.21}$$

The Schrödinger equation thus simplified reads

$$-\frac{1}{2}\frac{\mathrm{d}^2\varphi_n(u)}{\mathrm{d}u^2}+\frac{1}{2}u^2\varphi_n(u)=e_n\varphi_n(u). \tag{4.22}$$

This equation must be supplemented with the boundary conditions

$$\varphi_n(\pm\infty)=0. \tag{4.23}$$

The eigenfunctions and eigenvalues are of the form

$$\varphi_n(x)=N_n\exp\left(-\frac{1}{2}u^2\right)H_n(u), \qquad e_n=n+\frac{1}{2}. \tag{4.24}$$

The H_n are Hermite polynomials[3] of degree $n=0,1,2,\ldots$. The eigenfunctions and eigenvalues are also labeled by the quantum number n. Up to a phase, the constants N_n are obtained from the normalization condition (4.14)

$$N_n=2^{n/2}\left(\pi^{\frac{1}{2}}n!x_{\mathrm{c}}\right)^{-1/2}. \tag{4.25}$$

Since the Hamiltonian is a Hermitian operator, the eigenfunctions are orthogonal to each other and constitute a complete set of states:

[3]The reader is encouraged to verify that the few cases listed in Table 4.1 are correct solutions. Use can be made of the integrals

$$\int_{-\infty}^{\infty}\exp(-u^2)u^{2n}\mathrm{d}u=\frac{(2n-1)!!}{2^n}\pi^{\frac{1}{2}}, \qquad \int_{-\infty}^{\infty}\exp(-u^2)u^{2n+1}\mathrm{d}u=0.$$

Table 4.1 Solutions to the harmonic oscillator problem for small values of n. P_n is defined in (4.30)

n	e_n	H_n	$N_n \pi^{1/4} x_c^{1/2}$	P_n(%)
0	1/2	1	1	15.7
1	3/2	u	$\sqrt{2}$	11.2
2	5/2	$u^2 - 1/2$	$\sqrt{2}$	9.5
5	11/2	$u^5 - 5u^3 + 15u/4$	$2/\sqrt{15}$	5.7

$$\langle n|m\rangle = \int_{-\infty}^{\infty} \varphi_n^* \varphi_m \mathrm{d}x = \delta_{nm}, \qquad \Psi(x) = \sum_n c_n \varphi_n. \tag{4.26}$$

The solutions corresponding to the lower quantum numbers are displayed in Table 4.1 and Fig. 4.2.

4.2.2 Spatial Features of the Solutions

The following features arise from the spatial dimension associated with the Schrödinger formulation:

- *Probability density*. There are nodes in the probability density (except for the $n = 0$ state). The existence of such nodes is incompatible with the classical notion of a trajectory $x(t)$, according to which the particle bounces from one side of the potential to the other, while going through every intermediate point. The fact is that the particle can never be found at the nodes. The quantum picture reminds us of the stationary wave patterns obtained, for instance, inside an organ pipe. The role that is played in the case of sound by the ends of the pipe is played in the case of the quantum harmonic oscillator by the boundary conditions.
- *Comparison between the classical and quantum mechanical probability densities.* The classical probability for finding a particle is inversely proportional to its speed [$v = \left(2E/M - \omega^2 x^2\right)^{1/2}$ for the harmonic oscillator]. Therefore, we may define a classical probability density $P_{\mathrm{clas}} = \omega/\pi v$. The probability of finding the particle in any place, within the classically allowed interval $-x_n \le x \le x_n$, is 1. Here, $x_n = x_c(2n + 1)^{1/2}$ for a particle with energy $\hbar\omega(n + 1/2)$. The classical probability density displays a minimum around the origin and diverges as the particle approaches the end points of the allowed interval. The quantum mechanical density distribution for the ground state has exactly the opposite features. However, as n increases, the quantum mechanical density distribution tends towards the classical limit (Fig. 4.2). In fact, the quantum probability $P_n(x_0, \Delta x)$ satisfies the limiting relation

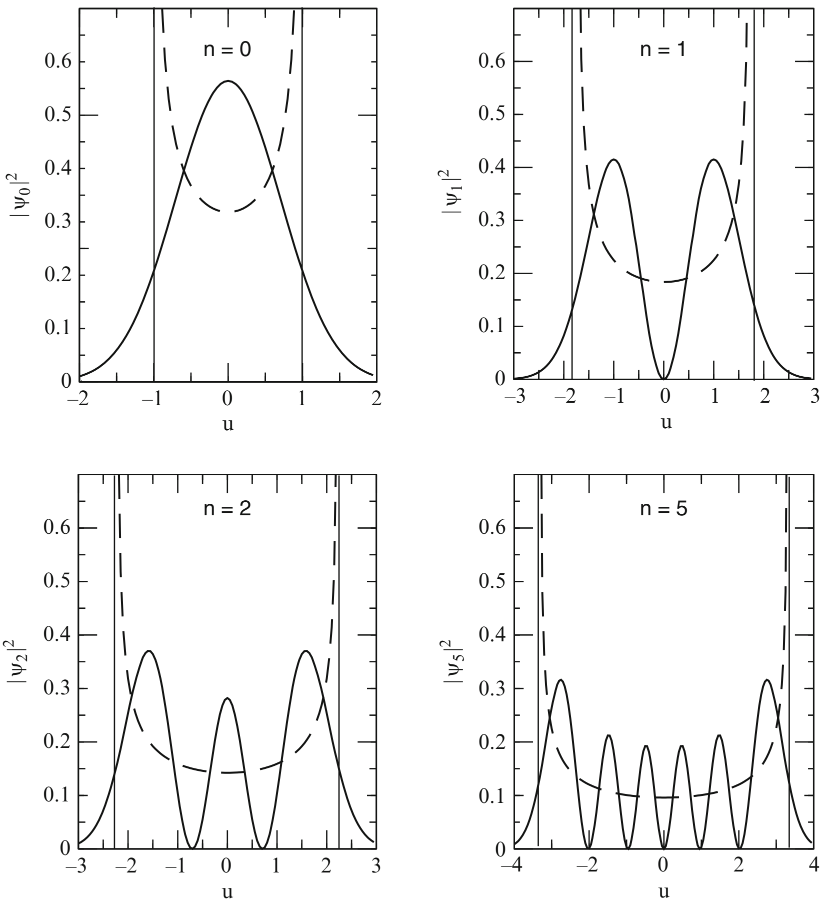

Fig. 4.2 Quantum mechanical probability densities and the classical probability densities of a harmonic oscillator potential as a function of the dimensionless distance u, for the quantum numbers $n = 0, 1, 2$ and 5. *Vertical lines* represent the limits of the classically allowed interval

$$\lim_{n\to\infty} P_n(x_0, \Delta x) = P_{\text{clas}}(x_0, \Delta x)$$

$$P_n(x_0, \Delta x) = \int_{x_0-\Delta x/2}^{x_0+\Delta x/2} |\varphi_n|^2 \mathrm{d}x, \tag{4.27}$$

as required by Bohr's correspondence principle.

- *Tunnel effect.* Outside the allowed interval $-x_c \leq x \leq x_c$, the classical particle would have a negative kinetic energy and thus an imaginary momentum. However, this argument does not hold in the quantum case, because it would imply some simultaneous determination of the particle location and the momentum, contradicting the uncertainty principle. Let us suppose that a particle in its ground state has been detected within the interval $x_c \le x \le \sqrt{2}x_c$, i.e. within the region following the classically allowed one. In this interval, the probability density decreases from N_0^2/e at $x = x_c$ to N_0^2/e^3 (i.e. by a factor e^{-2}). If we measure the particle within this interval, and we take it to be a reasonable measure of the uncertainty in the position of the particle, then

$$\Delta x \approx 0.41 x_c. \tag{4.28}$$

According to the Heisenberg principle, the minimum uncertainty in the determination of the momentum is

$$\Delta p \ge 1.22\sqrt{\hbar\omega M}, \tag{4.29}$$

which is consistent with an uncertainty in the kinetic energy larger than $(\Delta p)^2/2M \ge \frac{3}{4}\hbar\omega$. Since the potential energy in the same interval increases from $\hbar\omega/2$ to $\hbar\omega$, we cannot make any statement about a possible imaginary value for the momentum, which would rule out the possibility that the particle penetrates into the classically forbidden region.

The probability of finding the particle in the classically forbidden region is

$$P_n = \frac{2^{n+1}}{\pi^{1/2} n!}\int_{\sqrt{2n+1}}^{\infty} e^{-u^2}|H_n|^2 du. \tag{4.30}$$

This probability is a finite number, as large as 16% for the ground state. It decreases as the quantum number n increases, consistent with the tendency to approach the classical behavior for higher values of the energy (see Table 4.1).

4.3 Free Particle

If there are no forces acting on the particle, the potential is constant: $V(x) = V_0$. Let us assume in the first place that the energy $E \ge V_0$. In such a case the Schrödinger equation reads

$$-\frac{\hbar^2}{2M}\frac{d^2\varphi_k(x)}{dx^2} = (E - V_0)\varphi_k(x). \tag{4.31}$$

There are two independent solutions to this equation, namely

$$\varphi_{\pm k}(x) = A\exp(\pm ikx), \qquad k = \frac{\sqrt{2M(E-V_0)}}{\hbar}. \tag{4.32}$$

The parameter k labeling the eigenfunction is called the wave number and has dimensions of a reciprocal length. The eigenvalues of the energy and the momentum are

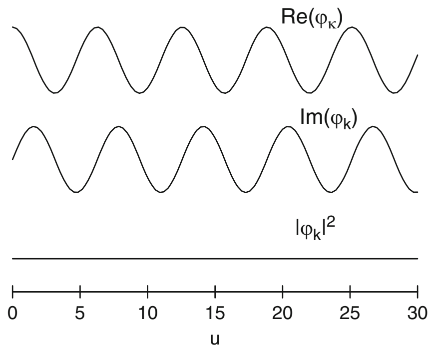

Fig. 4.3 Real component, imaginary component and modulus squared of a plane wave as functions of the dimensionless variable $u = kx$, where u is measured in radians

$$E = \hbar^2 k^2/2M + V_0, \qquad p = \pm\hbar k. \tag{4.33}$$

Unlike the case of the harmonic oscillator (a typical bound case), the eigenvalues of both the momentum and the energy belong to a continuous set. The free-particle solutions satisfy the de Broglie relation [32]

$$p = \hbar k = h/\lambda, \tag{4.34}$$

where λ is the particle wave length. The probability density is constant over the whole space (Fig. 4.3)

$$\rho_{\pm k}(x) = \varphi^*_{\pm k}(x)\varphi_{\pm k}(x) = |A|^2, \tag{4.35}$$

while the probability current reads

$$j_{\pm k}(x) = -\mathrm{i}\frac{\hbar}{2M}\left[\varphi^*_{\pm k}\frac{\mathrm{d}\varphi_{\pm k}(x)}{\mathrm{d}x} - \varphi_{\pm k}(x)\frac{\mathrm{d}\varphi^*_{\pm k}(x)}{\mathrm{d}x}\right] = \pm\frac{|A|^2\hbar k}{M}. \tag{4.36}$$

These results pose normalization problems, which may be

- Solved by applying more advanced mathematical tools, as in Sect. 11.1†
- Taken care of through the use of tricks, as in Sect. 4.4.1
- Circumvented, by looking only at the ratios of the probabilities of finding the particle in different regions of space (Sects. 4.5.1 and 4.5.2)

Since there are two degenerate solutions,[4] the most general solution for a given energy E is a linear combination

$$\Psi(x) = A_+ \exp(\mathrm{i}kx) + A_- \exp(-\mathrm{i}kx). \tag{4.37}$$

[4]Two or more solutions are called degenerate if they are linearly independent and have the same energy.

Let us consider now the case $E \le V_0$, which makes no sense from the classical point of view. However, the solution of the harmonic oscillator problem (third item in Sect. 4.2.2) has warned us not to reject this situation out of hand in the quantum case. In fact, the general solution is the linear combination[5]

$$\Psi(x) = B_+ \exp(\kappa x) + B_- \exp(-\kappa x), \qquad \kappa = -\mathrm{i}k = \frac{\sqrt{2M(V_0 - E)}}{\hbar}. \quad (4.38)$$

This general solution diverges at infinity: $|\Psi| \to \infty$ as $x \to \pm\infty$. Rather than a total rejection, this feature implies that the solution (4.38) can only be used if at least one of the extremes cannot be reached. For instance, if $V_0 > E$ for $x > a$, one imposes $B_+ = 0$.

4.4 One-Dimensional Bound Problems

4.4.1 Infinite Square Well Potential. Electron Gas

The potential in this case is $V(x) = 0$ if $|x| \le a/2$ and $V(x) = \infty$ for $|x| \ge a/2$ (Fig. 4.4).

The two infinite discontinuities should be canceled in the Schrödinger equation by similar discontinuities in the second derivative at the same points. This is accomplished by requiring the wave function to be a continuous function and requiring the first derivative to have a finite discontinuity at the boundaries of the potential. Since the wave function vanishes outside the classically allowed interval, the continuity of the wave function requires $\Psi(\pm a/2) = 0$.

According to (3.48), we may demand that the eigenfunctions of the Hamiltonian carry a definite parity. This is accomplished by using the solutions (4.37) with $A_+ = A_-$ for the even parity states, and $A_+ = -A_-$ for the odd ones. The eigenfunctions are written as

$$\varphi_n^{\text{even}}(x) = \sqrt{\frac{2}{a}} \cos(k_n x), \qquad \varphi_n^{\text{odd}}(x) = \sqrt{\frac{2}{a}} \sin(k_n x) \quad (4.39)$$

inside the well, and vanish outside the well. As a consequence of the boundary conditions,

$$\frac{k_n a}{2\pi} = n', \qquad n' = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots, \quad (4.40)$$

where the half-integer values correspond to the even solutions and the integer values to the odd ones. The eigenvalues of the energy are

[5] The only difference between the two solutions (4.37) and (4.38) is whether k is real or imaginary.

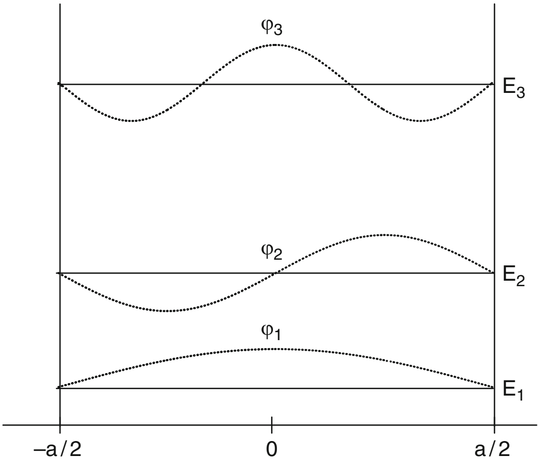

Fig. 4.4 Infinite square well potential. The energies E_n (*continuous lines*) and wave functions $\varphi_n(x)$ (*dotted curves*) are represented for the quantum numbers $n = 1, 2$ and 3

$$E_n = \frac{\hbar^2 k_n^2}{2M} = \frac{\hbar^2 \pi^2}{2Ma^2} n^2, \tag{4.41}$$

with $n = 2n' = 1, 2, \ldots$.

The reader is recommended to check that the quantum features associated with the solution of the harmonic oscillator problem (Sect. 4.2.2) are reproduced in the case of the infinite square well. The exception is the one related to the tunnel effect, which is prevented here by the infinite discontinuity in the potential.

By increasing the size of the box, the infinite potential well may be used to model the potential binding the electrons in a metal. In the electron gas model in one dimension, the (non-interacting) electrons are confined to a (large) segment a, which is much larger than the size of a given experimental set-up.

However, the standing waves (4.39) are not convenient for discussing charge and energy transport by electrons. In fact, the probability current associated with them vanishes. In the theory of metals, it is more convenient to use running waves $\exp(\pm ikx)$ (4.32). We may use an alternative boundary condition by imagining that the end point at $x = a/2$ is joined to the opposite point at $x = -a/2$. In this way the segment transforms into a circumference with the same length a. An electron arriving at the end of the well is not reflected back in, but leaves the metal and simultaneously re-enters at the opposite end. The representation of a free particle becomes more adequate as the radius $a/2\pi$ gets larger. This procedure results in the boundary condition $\Psi(x) = \Psi(x + a)$, or

$$\frac{k_n a}{2\pi} = n, \qquad n = 0, \pm 1, \pm 2, \ldots. \tag{4.42}$$

The total number of states is the same as for the standing waves (4.40), since the presence of half-integer and integer numbers in that case is compensated for here by the existence of two degenerate states $\pm n$. The eigenfunctions and energy eigenvalues are

$$\varphi_n(x) = \frac{1}{\sqrt{a}} \exp(\mathrm{i}k_n x), \qquad E_n = \frac{\hbar^2 k_n^2}{2M}. \tag{4.43}$$

As mentioned in Sect. 4.3, these functions are also eigenfunctions of the momentum operator $\hat{p}$ with eigenvalues $\hbar k_n$. Although the momenta (and the energies) are discretized, the gap

$$\Delta k = 2\pi/a \tag{4.44}$$

between two consecutive eigenvalues becomes smaller than any prescribed interval, if the radius of the circumference is taken to be sufficiently large.

In quantum mechanics, sums over intermediate states often appear. In the case of wave functions of the type (4.43), this procedure may be simplified by transforming the sums into integrals, using the length element in the integrals $(a/2\pi)\mathrm{d}k$, according to (4.44):

$$\sum_k f_k \to \frac{a}{2\pi} \int f_k \mathrm{d}k. \tag{4.45}$$

The extension of the model to include a periodic crystal structure is performed in Sect. 4.6[†]. Calculations with the electron gas model for the three-dimensional case are carried out in Sect. 7.4.1.

4.4.2 Finite Square Well Potential

The potential reads $V(x) = -V_0 < 0$ if $|x| < a/2$ and $V(x) = 0$ for other values of x. Here we consider only bound states, with a negative energy $(0 \geq -E \geq -V_0)$.

As in the harmonic oscillator case, the potential is invariant under the parity transformation $x \to -x$. Thus we expect the eigenfunctions to be either even or odd with respect to this transformation. Therefore, the solution (4.37) applies in the region $|x| \leq a/2$, with

$$A_+ = \pm A_- \quad \text{and} \quad k = \frac{1}{\hbar}\left[2M(V_0 - E)\right]^{1/2}.$$

Moreover, invariance under the parity transformation allows one to confine calculation of the boundary conditions to the position $x = a/2$. The wave function to the right of this point is given by (4.38) with $B_+ = 0$ and $\kappa = (1/\hbar)(2ME)^{1/2}$.

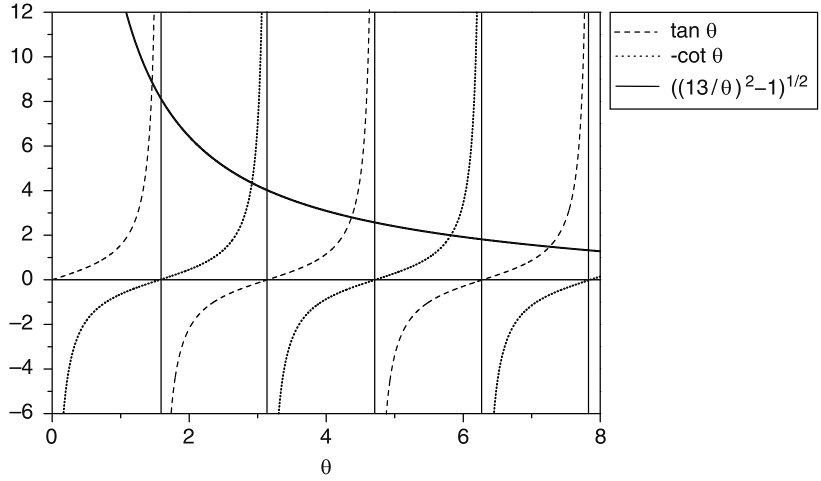

Fig. 4.5 Graphical determination of the energy eigenvalues of a finite square well potential. The intersections of the *continuous curve* $\sqrt{(13/\theta)^2 - 1}$ with the *dashed curves* correspond to even-parity solutions, while those with the *dotted curves* correspond to the odd ones. The value $MV_0a^2/\hbar^2 = 338$ is assumed

The ratio between the continuity conditions corresponding to the first derivative and to the function itself yields the eigenvalue equation

$$\frac{\kappa}{k} = \tan\frac{ka}{2}. \tag{4.46}$$

This is as far as we can go analytically in this case. Equation (4.46) must either be solved numerically or using the following graphical method: the equation determining the value of k is equivalent to the equation $E = V_0 - \hbar^2k^2/2M$. Therefore, we obtain the ratio

$$\frac{\kappa}{k} = \sqrt{\frac{2MV_0}{\hbar^2k^2} - 1}, \tag{4.47}$$

and (4.46) becomes

$$\sqrt{\frac{MV_0a^2}{2\hbar^2\theta^2} - 1} = \tan\theta, \tag{4.48}$$

where $\theta \equiv ka/2$. The function $\tan\theta$ increases from zero to infinity in the interval $0 \leq \theta \leq \pi/2$, while the left-hand side decreases from infinity to a finite value as θ increases in the same interval. Therefore, there is a value of θ at which the two curves intersect, corresponding to the lowest eigenvalue. An analogous argument is made for the successive roots of (4.48). The nth root is found in the interval $(n-1)\pi \leq \theta \leq (n-1/2)\pi$. (Fig. 4.5).

Unlike the harmonic oscillator case, the number of roots is limited, since (4.48) requires $\theta \leq \theta_{\max}$, where

$$\theta_{\max} = \sqrt{\frac{M V_0 a^2}{2\hbar^2}}. \tag{4.49}$$

There is a set of odd solutions that satisfy an equation similar to (4.46), namely

$$-\cot \frac{ka}{2} = \frac{\kappa}{k}. \tag{4.50}$$

Unlike the classical case, the probability density is not constant in the interval $|x| \leq a/2$. Moreover, there is a finite probability of finding the particle outside the classically allowed region. However, the solutions tend towards the classical behavior as n increases.

The spectrum of normalizable (bound) states is always discrete. Conversely, states that have a finite amplitude at infinity must be part of a continuous spectrum. This is the case for positive values of the energy (see Sect. 4.5.2).

4.5 One-Dimensional Unbound Problems

In this section we study problems related to the scattering of a particle by means of a potential. We assume that the particle impinges from the left and may be reflected and/or transmitted. There is no incoming wave from the right. Therefore the state vector must satisfy the following boundary conditions:

- It includes the term $A_+ \exp(\mathrm{i}kx)$ for $x \to -\infty$;
- It does not include the term $A_- \exp(-\mathrm{i}kx)$ for $x \to \infty$.

4.5.1 *One-Step Potential*

The one-step potential is written as $V(x) = 0$ for $x < 0$ and $V(x) = V_0 > 0$ for $x > 0$ (Fig. 4.6). It represents an electron moving along a conducting wire that is interrupted by a short gap. The electron feels a change in the potential as it crosses the gap.

$E_a < V_0$

Classically, the particle rebounds at $x = 0$ and cannot penetrate the region $x \geq 0$. Quantum mechanically this is no longer the case. For $x \leq 0$ the solution is given as the superposition of an incoming and a reflected wave (4.37), with $V_0 = 0$. Equation

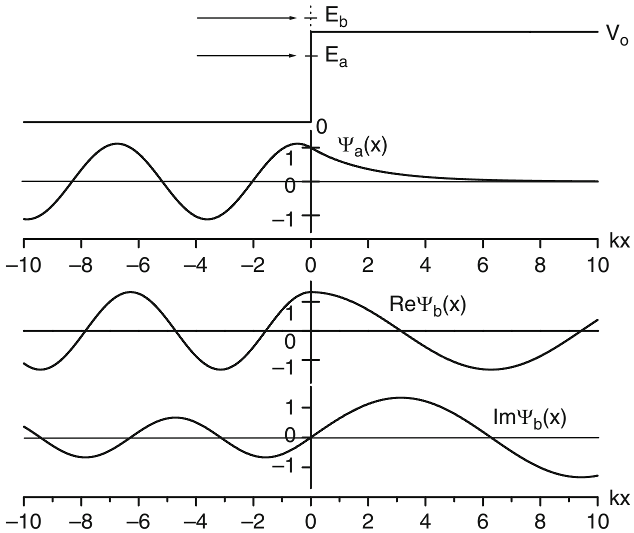

Fig. 4.6 One-step potential. Subscripts a and b label wave functions corresponding to energies $E_a = 3V_0/4$ and $E_b = 5V_0/4$, respectively

(4.38) holds for $x \geq 0$. This last solution cannot be rejected, since it does not diverge on the right half-axis if we impose the boundary condition $B_+ = 0$.

To have a Schrödinger equation valid at every point of space, the wave function and its first derivative should be continuous everywhere, including the point at which there is a finite discontinuity in the potential. These two requirements imply that

$$A_+ + A_- = B_- \,, \qquad A_+ - A_- = \mathrm{i}\frac{\kappa}{k} B_- . \tag{4.51}$$

Therefore

$$A_+ = \frac{1}{2} B_- \left(1 + \mathrm{i}\frac{\kappa}{k}\right), \qquad A_- = \frac{1}{2} B_- \left(1 - \mathrm{i}\frac{\kappa}{k}\right). \tag{4.52}$$

The total wave function is given by

$$\begin{aligned}\Psi_a(x) &= \frac{1}{2} B_- \left[\left(1 + \mathrm{i}\frac{\kappa}{k}\right) \exp(\mathrm{i}kx) + \left(1 - \mathrm{i}\frac{\kappa}{k}\right) \exp(-\mathrm{i}kx)\right] \\ &= B_- \left[\cos(kx) - \frac{\kappa}{k} \sin(kx)\right] \qquad (x \leq 0), \\ \Psi_a(x) &= B_- \exp(-\kappa x) \qquad (x \geq 0).\end{aligned} \tag{4.53}$$

The solution for $x \leq 0$ represents the superposition of an incident and a reflected wave. Since both amplitudes have equal module, they generate a standing wave with the corresponding nodes at positions such that $\tan(kx) = k/\kappa$, for $x \leq 0$ (see the first item in Sect. 4.2.2). The probability currents associated with the incident and reflected waves are

$$j_{\rm I} = -j_{\rm R} = \frac{\hbar k}{M}\frac{|B_-|^2}{4}\left(1+\frac{\kappa^2}{k^2}\right). \tag{4.54}$$

The reflection coefficient is defined as the absolute value of the ratio between reflected and incident currents. In the present case,

$$R \equiv \left|\frac{j_{\rm R}}{j_{\rm I}}\right| = 1. \tag{4.55}$$

The mutual cancelation between the two probability currents is correlated with the real character of the wave function (4.53).

There is a tunneling effect for $x \geq 0$, since the particle can penetrate into the forbidden region over a distance of the order of $\Delta x = 1/\kappa$. This length is accompanied by an uncertainty in the momentum and in the kinetic energy, so that

$$\Delta p \approx \frac{\hbar}{\Delta x} \approx \sqrt{2M(V_0 - E_a)}, \qquad \Delta E \approx \frac{(\Delta p)^2}{2M} \approx V_0 - E_a, \tag{4.56}$$

respectively. The consequences of these uncertainties parallel those discussed in Sect. 4.2.2.

$E_b > V_0$

The classical solution describes an incident particle which is totally transmitted, but with a smaller velocity. From the quantum mechanical point of view, the solution for $x \leq 0$ is again given by (4.37) with $V_0 = 0$, representing an incident plus a reflected wave. For $x \geq 0$ this same solution is valid, but with the wave number $k_b = \sqrt{2M(E_b - V_0)}/\hbar$. There is no incident wave from the right, since there is nothing that may bounce the particle back. Let C denote the amplitude of the transmitted wave $\exp(\mathrm{i}k_b x)$. The continuity of the wave function and its first derivative at $x = 0$ requires that

$$A_+ + A_- = C\ , \qquad A_+ - A_- = \frac{k_b}{k}C. \tag{4.57}$$

Using these equations, we may express the amplitudes of the reflected and transmitted waves as proportional to the amplitude of the incident wave, so that

$$\Psi_b(x) = \begin{cases} A_+\left[\exp(\mathrm{i}kx) + \dfrac{k-k_b}{k+k_b}\exp(-\mathrm{i}kx)\right] & (x \leq 0)\ , \\ A_+\dfrac{2k}{k+k_b}\exp(\mathrm{i}k_b x) & (x \geq 0). \end{cases} \tag{4.58}$$

The probability currents associated with the incident, reflected and transmitted waves are

$$\begin{aligned} j_{\rm I} &= \frac{\hbar k}{M}|A_+|^2, \\ j_{\rm R} &= -\frac{\hbar k}{M}\left(\frac{k-k_b}{k+k_b}\right)^2|A_+|^2, \\ j_{\rm T} &= \frac{\hbar k_b}{M}\left(\frac{2k}{k+k_b}\right)^2|A_+|^2, \end{aligned} \tag{4.59}$$

respectively. In this case we also define a transmission coefficient $T \equiv j_{\rm T}/j_{\rm I}$

$$R = \left(\frac{k-k_b}{k+k_b}\right)^2, \qquad T = \frac{4kk_b}{(k+k_b)^2}, \tag{4.60}$$

and we find that $R + T = 1$ as expected, since the current should be conserved in the present case.

What makes the particle bounce? The quantum mechanical situation is similar to a beam of light crossing the boundary between two media with different indices of refraction. At least a partial reflection of the beam takes place.

Note that the wave functions (4.53) and (4.58) may be obtained from each other through the substitution $k_b(E) = {\rm i}\kappa(E)$.

4.5.2 Square Barrier

The potential is given by $V(x) = 0$ ($|x| > a/2$) and $V(x) = V_0$ ($|x| < a/2$) (Fig. 4.7). We only consider explicitly the case $E \le V_0$. Classically, the particle can only be reflected at $x = -a/2$.

For $x \le -a/2$ and for $x \ge a/2$, the solution to the Schrödinger equation again takes the form (4.37), with the same value of k for both regions ($V_0 = 0$). However, there is only a transmitted wave, $C\exp({\rm i}kx)$, for $x \ge a/2$. Within the intermediate region $-a/2 \le x \le a/2$, the solution is as in (4.38). We cannot now reject either of the two components on account of their bad behavior at infinity. We thus have five amplitudes. The continuity conditions at the two boundaries provide us with four equations: the four remaining amplitudes may be expressed in terms of the amplitude of the incident wave A_+. We may also obtain here the currents associated with the incident beam $j_{\rm I}$, the reflected beam $j_{\rm R}$, the transmitted beam $j_{\rm T}$ and the beam within the barrier $j_{\rm B}$, and the reflection and transmission coefficients R, T:

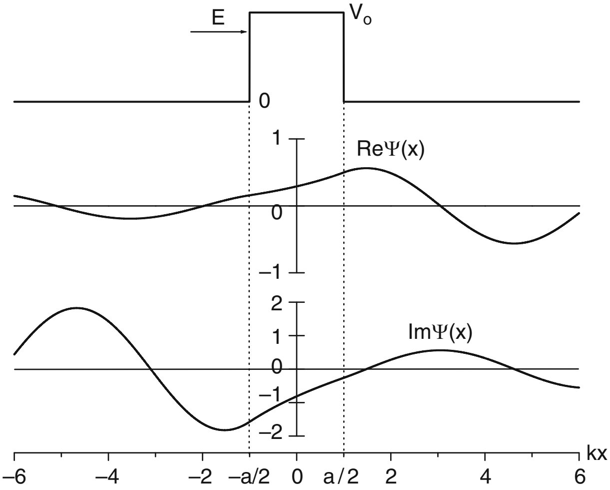

Fig. 4.7 Square barrier and associated wave function. Here $E = 3V_0/4$

$$j_{\rm I} = \frac{\hbar k}{M}|A_+|^2, \qquad j_{\rm R} = -\frac{\hbar k}{M}|A_-|^2,$$

$$j_{\rm T} = \frac{\hbar k}{M}|C|^2, \qquad j_{\rm B} = \frac{2\hbar\kappa}{M}\Big[\mathrm{Re}\,(B_+)\mathrm{Im}\,(B_-) - \mathrm{Re}\,(B_-)\mathrm{Im}\,(B_+)\Big],$$

$$R = \left|\frac{j_{\rm R}}{j_{\rm I}}\right| = \frac{\sinh^2(\kappa a)}{\dfrac{4E}{V_0}\left(1-\dfrac{E}{V_0}\right) + \sinh^2(\kappa a)},$$

$$T = \left|\frac{j_{\rm T}}{j_{\rm I}}\right| = \left|\frac{j_{\rm B}}{j_{\rm I}}\right| = \frac{\dfrac{4E}{V_0}\left(1-\dfrac{E}{V_0}\right)}{\dfrac{4E}{V_0}\left(1-\dfrac{E}{V_0}\right) + \sinh^2(\kappa a)}. \tag{4.61}$$

For values of $\kappa a > 1$ the transmission coefficient displays an exponential decay

$$T \approx \frac{16E}{V_0}\left(1-\frac{E}{V_0}\right)\exp(-2\kappa a). \tag{4.62}$$

Transmission through a potential barrier is another manifestation of the tunnel effect, which has been discussed both in connection with the harmonic oscillator (Sect. 4.2.2) and with the one-step potential (Sect. 4.5.1). The tunnel effect manifests itself in the α-decay of nuclei, the tunneling microscope, etc.

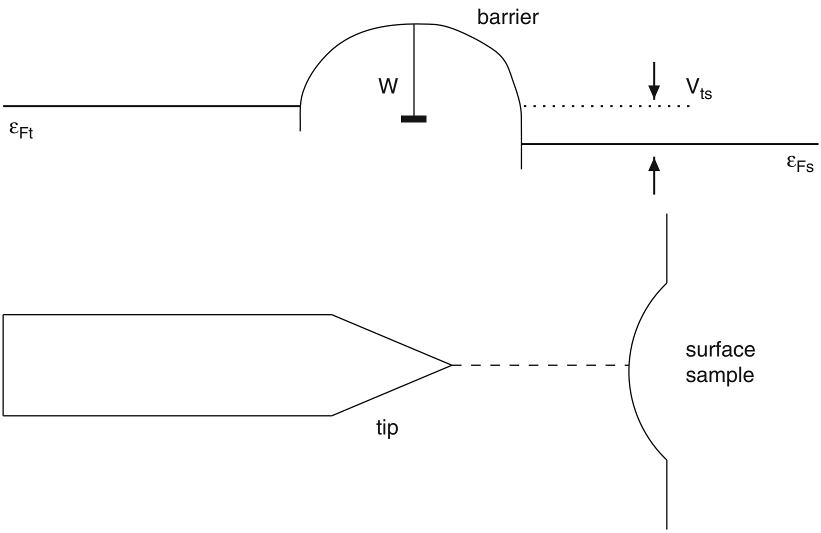

Fig. 4.8 Scanning tunneling microscope

The corresponding analysis for the case of a potential well parallels the one made for the square barrier. A solution of type (4.37), instead of (4.38), should also be used for the region inside the well. There will also be incident, reflected and transmitted waves, and coefficients of reflection and transmission that sum to a value of unity.

4.5.3 Scanning Tunneling Microscope

The scanning tunneling microscope (STM) was developed in the 1980s by Gerd Binnig and Heinrich Rohrer [33]. A conducting probe ending in a very sharp tip is held close to a metal sample. In a metal, electrons move freely according to the electron gas model [Sects. (4.4.1) and (7.4.1)], filling all levels up to the Fermi energy ϵ_F. The potential rises at the surface of the metal forming a barrier, and electrons tunnel through the barrier between tip and surface sample (Fig. 4.8). The tunneling current[6] is proportional to the transmission coefficient T (4.62). Thus, it exponentially increases as the distance tip–surface decreases. The tip is mounted on a piezoelectric tube, which allows very small movements by applying voltage at its electrodes. The tip slowly scans the surface.

[6] A small voltage difference V_{ts} between tip and sample must be introduced, to ensure the existence of empty electron states in the sample, that should be occupied by tunneled electrons.

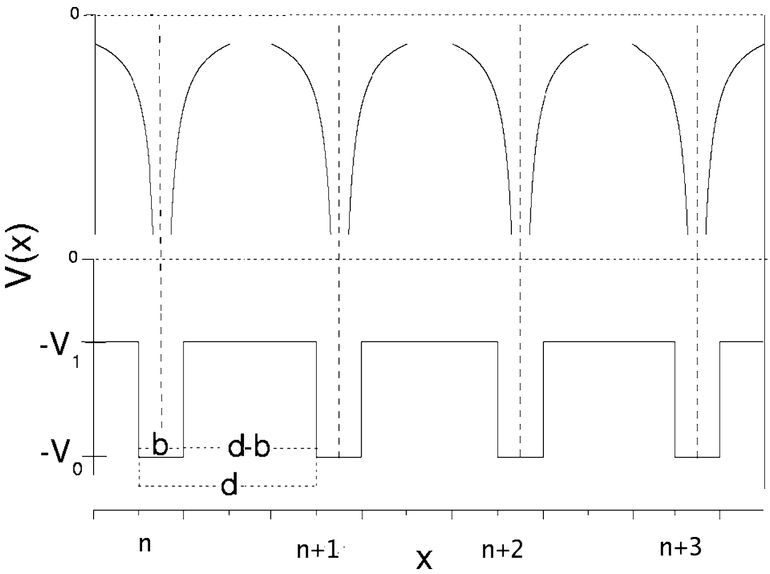

Fig. 4.9 Periodic potential. The upper part of the figure represents a realistic potential. The lower one mocks this potential as successive square wells

An effective value of κ can be estimated by replacing the difference $V_0 - E$ in (4.38) by an average of sample and tip work functions W (the smallest energy needed to remove an electron from a metal, about 4 eV). Thus $\kappa \approx 2\,\text{Å}^{-1}$ and, consequently, the device is sensitive to changes in distance at the subangstrom scale (Problem 12).

The tip is moved over the surface of the sample, which requires high precision movement coupled to electrical control. This is achieved by means of piezoelectric elements.

The STM is used in both industrial and basic research to obtain atomic-scale images of metal surfaces and of other materials, from the atomic to the micron scale. It is also possible to achieve tiny tunnel currents if, for instance, biological materials are spread as thin films over conductive substrates.

Large electric fields applied to the tip can lift atoms one by one and deposit them at chosen locations. The contents of all books from the British Library could thus fit on top of one stamp. One can also make small "quantum corrals," a few angstrom wide.[7]

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[7]However, it is still difficult to find quantum features in these small systems because of decoherence (see Sect. 14.2†).

4.6† Band Structure of Crystals

A crystal consists of an array of N positive ions displaying a periodic structure in space and electrons moving in the electric field generated by the ions. Figure 4.9 sketches the potential $V(x+d) = V(x)$ that an electron feels in the one-dimensional case. In this section we study the main features of the single-particle eigenstates in such a potential.

Classically, an electron moving in the potential of Fig. 4.9 may be bound to a single ion so that it is unable to transfer to another ion. Quantum mechanically, this may be ensured only if the distance d between the ions is very large. In such a case, the N states in which the electron is bound to one atom of the array constitute an orthogonal set of states which is N times degenerate. However, as the distance d is reduced to realistic values, we expect the degeneracy to be broken and the energy eigenvalues to be distributed within a band. In the following, we show how this picture is represented mathematically.

The Bloch theorem states that the wave function of a particle moving in a periodic potential has the form

$$\varphi_k(x) = \exp(\mathrm{i}kx)u_k(x), \tag{4.63}$$

where k is real and $u_k(x + d) = u_k(x)$ is a periodic function [34].

Since the most relevant property of the potential is its periodicity and not its detailed shape, we replace the realistic potential with a periodic array of square well potentials (Fig. 4.9). We have learned by now how to solve square well problems. Here $V(x) = -V_0$ $(0 \le x \le b)$ and $V(x) = -V_1$ $(b \le x \le d)$. Moreover, $V(x + d) = V(x)$. We denote the energy by $-E$, with $E > 0$. We assume that the electron is bound to the crystal for negative energy values.

Region I: $-V_0 \le -E \le -V_1$

According to Sect. 4.3, the wave functions in the interval $nd \le x \le (n + 1)d$ are

$$\Psi(x) = \begin{cases} A_+ \exp(\mathrm{i}k_b x) + A_- \exp(-\mathrm{i}k_b x), & nd \le x \le nd + b, \\ B_+ \exp(\kappa_b x) + B_- \exp(-\kappa_b x), & nd + b \le x \le (n+1)d, \end{cases} \tag{4.64}$$

where

$$k_b = \frac{1}{\hbar}\sqrt{2M(V_0 - E)}, \qquad \kappa_b = \frac{1}{\hbar}\sqrt{2M(E - V_1)}. \tag{4.65}$$

Thus the periodic function $u_k(x)$ is of the form

$$u_k(x) = \begin{cases} A_+ \exp[\mathrm{i}(k_b - k)x] + A_- \exp[-\mathrm{i}(k_b + k)x], & nd \le x \le nd + b, \\ B_+ \exp[(\kappa_b - \mathrm{i}k)x] + B_- \exp[-(\kappa_b + \mathrm{i}k)x], & \\ & nd + b \le x \le (n+1)d. \end{cases} \tag{4.66}$$

The periodicity of u_k requires

$$u_k(x) = A_+ \exp[\mathrm{i}(k_b - k)(x-d)] + A_- \exp[-\mathrm{i}(k_b + k)(x-d)], \qquad (4.67)$$

for

$$(n+1)d \le x \le (n+1)d + b.$$

The continuity conditions for the wave function, or equivalently for u_k, yield four linear equations for the amplitudes $A_\pm, B_\pm$ (two at $x = b$ and two at $x = d$). Therefore the determinant of the coefficients of the amplitudes should vanish. This condition leads to the equation

$$f(E) = \cos(kd), \qquad (4.68)$$

where

$$f(E) = \frac{\kappa_b^2 - k_b^2}{2k_b\kappa_b} \sinh\left[\kappa_b(d-b)\right]\sin(k_b b) + \cosh\left[\kappa_b(d-b)\right]\cos(k_b b). \qquad (4.69)$$

Region II: $-V_1 \le -E \le 0$

The procedure is completely parallel to the previous case except for the fact that the wave function is also of the form (4.37) in the interatomic space $b \le x \le d$, with $k_c = (1/\hbar)\sqrt{2M(E - V_1)}$. Equation (4.68) still holds, with

$$f(E) = -\frac{k_c^2 + k_b^2}{2k_b k_c} \sin\left[k_c(b-d)\right]\sin(k_b b) + \cos\left[k_c(d-b)\right]\cos(k_b b). \qquad (4.70)$$

The allowed values of E fall into bands satisfying the condition $|f(E)| \le 1$. Figure 4.10 represents the function $f(E)$, encompassing the two regions I and II, for the parameters $V_1 = V_0/2$ and $b = \hbar\sqrt{2/MV_0}$.

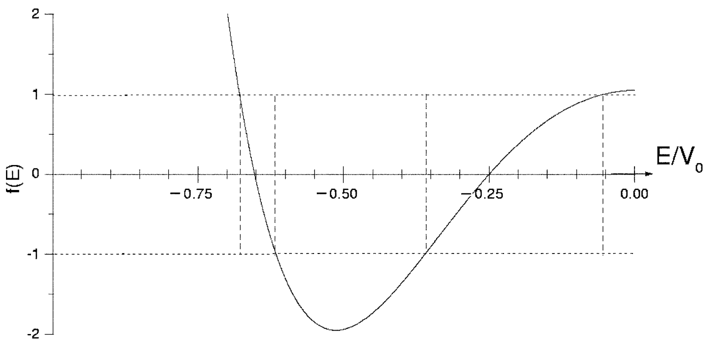

Fig. 4.10 Available intervals of energy (bands), obtained with the periodic square potential of Fig. 4.9

Equation (4.68) remains unchanged if k is increased by a multiple of $2\pi/d$. We therefore confine k to the interval

$$-\frac{\pi}{d} \leq k \leq \frac{\pi}{d}. \tag{4.71}$$

We now apply the periodic boundary conditions discussed in Sect. 4.4.1. The length of the circumference is $a = Nd$. Therefore,

$$\exp(\mathrm{i}k_n Nd) = 1, \qquad k_n = \pm\frac{2\pi n}{Nd}, \qquad n = 0, \pm 1, \pm 2, \pm\frac{1}{2}N, \tag{4.72}$$

where the limits (4.71) have been taken into account. There are as many possible values of k as there are ions in the array. This result is consistent with the fact that binding the electron to each ion also constitutes a possible solution to the problem, as mentioned at the beginning of this section.

Problems

Problem 1. Using Table 4.1, verify that

1. The operator a (3.29) annihilates the ground state wave function φ_0
2. The operator a^+, applied to $\varphi_1(x)$ yields $\sqrt{2}\varphi_2(x)$

Hint: express the operators a, a^+ as differential operators.

Problem 2. Assume an infinite square well such that $V(x) = 0$ in the interval $0 < x < a$ and $V(x) = \infty$ for the remaining values of x.

1. Calculate the energies and wave functions.
2. Compare these results with those obtained in the text centering the well at the origin and explain the agreement on physical grounds.
3. Do the wave functions obtained in the first part have a definite parity?

Problem 3. Relate the minimum energy for a particle moving in a square well to the Heisenberg uncertainty principle.

Problem 4. Find the eigenvalue equations for a particle moving in a potential well such that $V(x) = \infty$ for $|x| \geq a/2$, $V(x) = V_0 \geq 0$ for $-a/2 \leq x \leq 0$ and $V(x) = 0$ for $0 < x < a/2$. Assume $0 \leq E \leq V_0$.

Problem 5. Estimate the error if we use (4.45) in the calculation of $\sum_k E_k$. Hint: recall that

$$\sum_{n=0}^{n=\nu} n^2 = \frac{\nu}{6}(\nu + 1)(2\nu + 1).$$

Problem 6. Assume a free electron gas confined to a one-dimensional well of width a

1. Obtain the density of states $\rho(E)$ as a function of energy.
2. Calculate ρ for $E = 1\,\text{eV}$ and $a = 1\,\text{cm}$.

Problem 7. Consider a square well such that $V(x) = \infty$ for $x < 0$, $V(x) = 0$ for $0 < x < a/2$ and $V(x) = V_0$ for $x > a/2$.

1. Write down the equation for the eigenvalues.
2. Compare this equation with the one obtained for the finite square well in Sect. 4.4.2.
3. For $V_0 \rightarrow \infty$, show that the wave function for the finite well satisfies the condition that it vanishes at $x = a/2$ and does not penetrate the classically forbidden region.

Problem 8. Calculate the number of even-parity states (EPS) and odd parity states (OPS) for a finite square well potential of depth V_0 centered at the origin, if the parameter

$$\theta = \frac{a}{\hbar}\sqrt{\frac{MV_0}{2}}$$

lies in the intervals $(0, \pi/2)$, $(0, \pi)$, $(0, 3\pi/2)$ and $(0, 2\pi)$.

Problem 9. Calculate the transmission and reflection coefficients for an electron with a kinetic energy of $E = 2\,\text{eV}$ coming from the right. The potential is $V(x) = 0$ for $x \leq 0$ and $V(x) = V_0 = 1\,\text{eV}$ for $x \geq 0$.

Problem 10. The highest energy of an electron inside a block of metal is 5 eV (Fermi energy). The additional energy that is necessary to remove the electron from the metal is 3 eV (work function).

1. Estimate the distance through which the electron penetrates the barrier, assuming that the width of the (square) barrier is much greater than the penetration distance.
2. Estimate the transmission coefficient if the width of the barrier is 20 Å.

Problem 11. Obtain the transmission coefficients of a potential barrier in the limits $\kappa a \ll 1$ and $\kappa a \gg 1$.

Problem 12. Estimate the sensitivity to the distance tip-sample in an STM, assuming that a relative variation of 1% in the current can be detected and $\kappa = 2\,\text{Å}^{-1}$.

Problem 13. 1. Show that the eigenfunction of the Hamiltonian of a periodic potential is not an eigenfunction of the momentum operator.
2. Why is it not a momentum eigenstate?
3. Give an expression for the expectation value of the momentum.

Problem 14. In the presence of interactions, it is sometimes useful to mock the spectrum by one of a free particle (4.33) with an effective mass. Obtain the value of M_{eff} at the extremes of the intervals allowed by (4.68).
Hint: Expand both sides of (4.68) and add the resulting expression $\Delta E(k^2)$ to the kinetic energy (4.33).

Problem 15. A linear combination $\Psi(x)$ of momentum eigenstates (4.43) representing a localized particle is called a wave packet. Choose as amplitudes $c_p = \eta \exp[-p^2/\alpha^2]$.

1. Obtain the value of η such that the normalization condition $\sum_p |c_p|^2 = 1$ is satisfied.
2. Calculate the probability density $|\Psi(x)|^2$.
3. Obtain the matrix elements $\langle\Psi|x|\Psi\rangle$ and $\langle\Psi|x^2|\Psi\rangle$.
4. Obtain the matrix elements $\langle\Psi|p|\Psi\rangle$ and $\langle\Psi|p^2|\Psi\rangle$.
5. Verify Heisenberg uncertainty relation (2.37).

Hint: replace sums by integrals as in (4.45).
$\int_{-\infty}^{\infty} \exp[-(x + \mathrm{i}\beta)^2/\alpha^2]\mathrm{d}x = \alpha\sqrt{\pi/2}$; $\quad \int_{-\infty}^{\infty} f(k)\exp[ikx]\mathrm{d}x = 2\pi f(0)$.