Chapter 3
Simple Model Systems

One-dimensional models and models with piecewise constant potentials have been used as simple model systems for quantum behavior ever since the inception of Schrödinger's equation. These models vary in their levels of sophistication, but their generic strength is the clear demonstration of important general quantum effects and effects of dimensionality of a quantum system at very little expense in terms of effort or computation. Simple model systems are therefore more than just pedagogical tools for teaching quantum mechanics. They also serve as work horses for the modeling of important quantum effects in nanoscience and technology, see e.g. [4, 20].

3.1 Barriers in quantum mechanics

Widely used models for quantum behavior in solid state electronics are described by piecewise constant potentials $V(\boldsymbol{x})$. This means that $V(\boldsymbol{x})$ attains constant values in different regions of space, and the transition between those regions of constant $V(\boldsymbol{x})$ appears through discontinuous jumps in the potential. Figure 3.1 shows an example of a piecewise constant potential.

The Schrödinger equation with a piecewise constant potential is easy to solve, and the solutions provide instructive examples for the impact of quantum effects on the motion of charge carriers through semiconductors and insulating barriers. We will first discuss the case of a rectangular barrier.

Figure 3.1 shows a cross section of a non-symmetric rectangular square barrier.

The piecewise constant potential has values

$$V(\boldsymbol{x}) = \begin{cases} 0, & x < 0, \\ \Phi_1, & 0 \leq x \leq L, \\ \Phi_2, & x > L. \end{cases}$$

© Springer International Publishing Switzerland 2016

R. Dick, *Advanced Quantum Mechanics*, Graduate Texts in Physics,
DOI 10.1007/978-3-319-25675-7_3

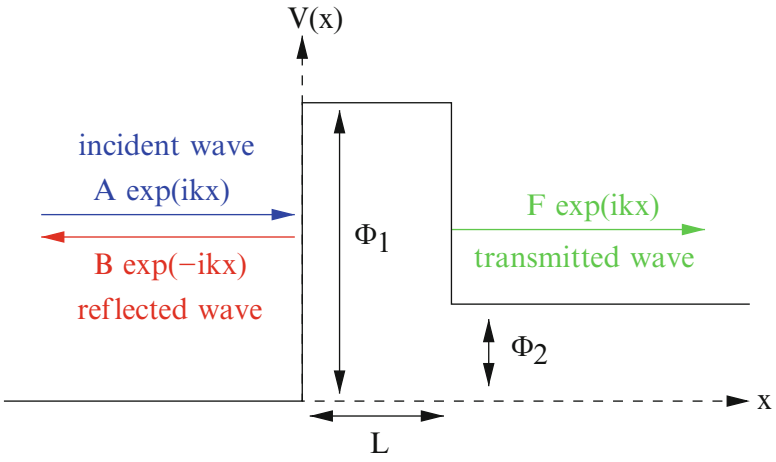

Fig. 3.1 A non-symmetric square barrier

with $\Phi_1 > \Phi_2 > 0$. This barrier impedes motion in the x direction. It can be used e.g. as a simple quantum mechanical model for a metal coated with an insulating layer. The region $x < 0$ would be inside the metal and the potential Φ_2 would be the energy which is required to liberate an electron from the metal if there would not be the insulating layer of thickness L. The energy Φ_1 is the energy which would classically be required for an electron to penetrate the layer.

Quantum problems with time-independent potentials are conveniently analyzed by using a Fourier transformation[1] from time t to energy E,

$$\psi(\boldsymbol{x},t) = \frac{1}{\sqrt{2\pi}\hbar}\int_{-\infty}^{\infty} dE\, \exp\left(-\frac{\mathrm{i}}{\hbar}Et\right)\psi(\boldsymbol{x},E), \tag{3.1}$$

$$\psi(\boldsymbol{x},E) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dt\, \exp\left(\frac{\mathrm{i}}{\hbar}Et\right)\psi(\boldsymbol{x},t). \tag{3.2}$$

Substitution into the time-dependent Schrödinger equation (1.2) yields the time-independent Schrödinger equation[2]

$$E\psi(\boldsymbol{x},E) = -\frac{\hbar^2}{2m}\Delta\psi(\boldsymbol{x},E) + V(\boldsymbol{x})\psi(\boldsymbol{x},E). \tag{3.3}$$

[1]The normalization condition (1.20) implies that the function $\psi(\boldsymbol{x},E)$ does not exist in the sense of classical Fourier theory. We will therefore see in Section 5.2 that $\psi(\boldsymbol{x},E)$ is rather a series of δ-functions of the energy. This difficulty is usually avoided by using an *exponential ansatz* $\psi(\boldsymbol{x},t) = \psi(\boldsymbol{x},E)\exp(-\mathrm{i}Et/\hbar)$ instead of a full Fourier transformation. However, if one accepts the δ-function and corresponding extensions of classical Fourier theory, the transition to the time-independent Schrödinger equation through a formal Fourier transformation to the energy variable is logically more satisfactory.

[2]E. Schrödinger, Annalen Phys. 384, 361 (1926). Schrödinger found the time-independent equation first and published the time-dependent equation (1.2) five months later.

The potential on Figure 3.1 depends only on x. In this case we can also eliminate the derivatives with respect to y and z through further Fourier transformations,

$$\psi(\boldsymbol{x}, E) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_2 \int_{-\infty}^{\infty} dk_3 \, \exp[\mathrm{i}(k_2 y + k_3 z)] \, \psi(x, k_2, k_3, E)$$

to find the time-independent Schrödinger equation for motion in the x direction,

$$E_1 \psi(x, E_1) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x, E_1) + V(x) \psi(x, E_1). \tag{3.4}$$

Here

$$E_1 \equiv E - \hbar^2 \frac{k_2^2 + k_3^2}{2m}, \quad \psi(x, E_1) \equiv \psi(x, k_2, k_3, E).$$

E_1 is the kinetic energy for motion in the x direction in the region $x < 0$.

Within each of the three separate regions $x < 0$, $0 < x < L$, and $x > L$ the potential attains a constant value, and equation (3.4) can be solved with a final Fourier transformation from x to k_1,

$$\psi(x, E_1) = \begin{cases} A \exp(\mathrm{i}k_1 x) + B \exp(-\mathrm{i}k_1 x), \;\; k_1 = \sqrt{2mE_1}/\hbar, \;\; x < 0, \\ C \exp(\mathrm{i}k_1'' x) + D \exp(-\mathrm{i}k_1'' x), \\ \quad k_1'' = \sqrt{2m(E_1 - \Phi_1)}/\hbar, \;\; 0 < x < L, \\ F \exp(\mathrm{i}k_1' x) + G \exp(-\mathrm{i}k_1' x), \\ \quad k_1' = \sqrt{2m(E_1 - \Phi_2)}/\hbar, \;\; x > L. \end{cases} \tag{3.5}$$

We must have $E_1 > 0$ because the absolute minimum of the potential determines a lower bound for the energy of a particle moving in the potential. However, the wave numbers k_1'' and k_1' can be real or imaginary depending on the magnitude of E_1. We define

$$k_1'' = -\mathrm{i}\kappa, \quad k_1' = \mathrm{i}\kappa',$$

with the conventions $\kappa > 0$, $\kappa' > 0$, if k_1'' or k_1' are imaginary.

The wave function (3.5) is not yet the complete solution to our problem, because we have to impose junction conditions on the coefficients at the transition points $x = 0$ and $x = L$ to ensure that the Schrödinger equation is also satisfied in those points. This will be done below. However, we can already discuss the meaning of the six different exponential terms appearing in (3.5). The wave function $\psi(x, E_1)$ is multiplied by the time-dependent exponential $\exp(-\mathrm{i}E_1 t/\hbar)$ in the transition from $\psi(x, E_1)$ to the time-dependent wave function $\psi(x, t)$ for motion in x direction,

$$\psi(x, t) = \frac{1}{\sqrt{2\pi\hbar}} \int_0^{\infty} dE_1 \, \exp\left(-\frac{\mathrm{i}}{\hbar} E_1 t\right) \psi(x, E_1). \tag{3.6}$$

A single monochromatic component therefore corresponds to a time-dependent wave function proportional to $\psi(x, E_1)\exp(-\mathrm{i}E_1 t/\hbar)$. The term $A\exp[\mathrm{i}(k_1 x - E_1 t/\hbar)]$ corresponds to a right moving wave in the region $x < 0$, while the term $B\exp[-\mathrm{i}(k_1 x + E_1 t/\hbar)]$ is a left moving wave. Similar identifications apply to the C and D components if k_1'' is real, and to the F and G components if k_1' is real. Otherwise, these components will correspond to exponentially damped or growing wave functions, which requires $G = 0$ if $\kappa' = -\mathrm{i}k_1' > 0$ is real, to avoid divergence of the wave function for $x \to \infty$.

There is a subtle point here that needs to be emphasized because it is also relevant for potential scattering theory in three dimensions. We have just realized that the monochromatic wave function $\psi(x, E_1)$ describes a particle of energy E_1 (for the motion in x direction) simultaneously as left and right moving particles in the regions where the wave number is real. The energy dependent wave function always simultaneously describes all states of the particle with energy E_1, but does not yield a time resolved picture of what happens to a particle in the presence of the potential $V(x)$. Let us e.g. assume that we shoot a particle of energy E_1 at the potential $V(x)$ from the left. The component $A\exp[\mathrm{i}(k_1 x - E_1 t/\hbar)]$ describes the initially incident particle, while the component $B\exp[-\mathrm{i}(k_1 x + E_1 t/\hbar)]$ describes a particle that is reflected by the barrier. The component $F\exp[\mathrm{i}(k_1' x - E_1 t/\hbar)]$, on the other hand, describes a particle which went across the barrier (if $E_1 > \Phi_1$), or a particle that penetrated the barrier (without damaging the barrier!) if $\Phi_1 > E_1 > \Phi_2$.

The calculation of expectation values sheds light on the property of the monochromatic wave function $\psi(x, E_1)\exp(-\mathrm{i}E_1 t/\hbar)$ to describe all states of a particle of energy E_1 simultaneously. The expectation values both for location $\langle x\rangle$ and momentum $\langle p\rangle$ of a particle described by a monochromatic wave function are time-independent, i.e. a single monochromatic wave function can never describe the time evolution of motion of a particle in the sense of first corresponding to an incident wave from the left, and later either to a reflected wave or a transmitted wave. A time resolved picture describing sequential events really requires superposition of several monochromatic components (3.6) with contributions from many different energies. Stated differently, the wave function of a moving particle can never correspond to only one exact value for the energy of the particle. Building wave functions for moving particles will always require superposition of different energy values, which corresponds to an uncertainty in the energy of the particle. Stated in yet another way: The energy resolved picture described by the Schrödinger equation in the energy domain (3.3) describes all processes happening with energy E, whereas the time-dependent Schrödinger equation describes processes happening at time t. If the time-dependent wave function of the system is indeed monochromatic, $\psi(x, t) = \psi(x, E_1)\exp(-\mathrm{i}E_1 t/\hbar)$, then we imply that all these processes at energy E_1 happen simultaneously, e.g. because we have a continuous particle beam of energy E_1 incident on the barrier.

The monochromatic wave function can still tell us a lot about the behavior of particles in the presence of the potential barrier $V(x)$. We choose as an initial condition a particle moving against the barrier from the left. Then we have to set $G = 0$ in the solution above irrespective of whether k_1' is real or imaginary, because

in the real case this component would correspond to a particle hitting the barrier from the right, and in the imaginary case $G = 0$ was imposed anyway from the requirement that the wave function cannot diverge.

Before we can proceed, we have to discuss junction conditions for wave functions at points where the potential is discontinuous.

A finite jump in $V(x)$ translates through the time-independent Schrödinger equation into a finite jump in $d^2\psi(x)/dx^2$, which means a jump in the slope of $d\psi(x)/dx$, but not a discontinuity in $d\psi(x)/dx$. Therefore both $\psi(x)$ and $d\psi(x)/dx$ have to remain continuous across a finite jump in the potential[3]. This means that the wave function $\psi(x)$ remains smooth across a finite jump in $V(x)$. On the other hand, an infinite jump in $V(x)$ only requires continuity, but not smoothness of $\psi(x)$.

The requirement of smoothness of the wave function yields the junction conditions

$$\begin{aligned} A + B &= C + D \\ k_1(A - B) &= k_1''(C - D) \\ C\exp(\mathrm{i}k_1''L) + D\exp(-\mathrm{i}k_1''L) &= F\exp(\mathrm{i}k_1'L) \\ k_1''[C\exp(\mathrm{i}k_1''L) - D\exp(-\mathrm{i}k_1''L)] &= k_1'F\exp(\mathrm{i}k_1'L) \end{aligned}$$

Elimination of C and D yields

$$\begin{aligned} 2k_1k_1''A &= \left[k_1''(k_1 + k_1')\cos(k_1''L) - \mathrm{i}(k_1k_1' + k_1''^2)\sin(k_1''L)\right]F\exp(\mathrm{i}k_1'L), \\ 2k_1k_1''B &= \left[k_1''(k_1 - k_1')\cos(k_1''L) - \mathrm{i}(k_1k_1' - k_1''^2)\sin(k_1''L)\right]F\exp(\mathrm{i}k_1'L). \end{aligned}$$

Note that

$$\cos(k_1''L) = \cosh(\kappa L), \quad \sin(k_1''L) = -\,\mathrm{i}\sinh(\kappa L).$$

If we decompose the wave function to the left and the right of the barrier into incoming, reflected, and transmitted components

$$\psi_{in}(x) = A\exp(\mathrm{i}k_1x), \quad \psi_{re}(x) = B\exp(-\mathrm{i}k_1x), \quad \psi_{tr}(x) = F\exp(\mathrm{i}k_1'x),$$

then the probability current density (1.18) yields

$$j_{in} = \frac{\hbar k_1}{m}|A|^2, \quad j_{re} = -\frac{\hbar k_1}{m}|B|^2, \quad j_{tr} = \frac{\hbar}{m}|F|^2\Re k_1'.$$

[3]The time-dependent Schrödinger equation permits discontinuous wave functions $\psi(x,t)$ even for smooth potentials, because there can be a trade-off between the derivative terms, see e.g. Problem 3.15.

In the last equation we used that k_1' is either real or imaginary. The reflection and transmission coefficients from the barrier are then

$$R = \frac{|j_{re}|}{|j_{in}|} = \frac{|B|^2}{|A|^2}, \quad T = \frac{|j_{tr}|}{|j_{in}|} = \frac{|F|^2 \Re k_1'}{|A|^2 k_1}.$$

This yields in all cases $0 \leq T = 1 - R \leq 1$. The transmission coefficient is $T = 0$ for $0 < E_1 \leq \Phi_2$,

$$\begin{aligned} T = {} & 4\sqrt{E_1(E_1 - \Phi_2)}(\Phi_1 - E_1) \\ & \times \Big[(\Phi_1 - E_1) \left(2E_1 - \Phi_2 + 2\sqrt{E_1(E_1 - \Phi_2)} \right) \\ & + \Phi_1(\Phi_1 - \Phi_2) \sinh^2\left(\sqrt{2m(\Phi_1 - E_1)} L/\hbar \right) \Big]^{-1} \end{aligned}$$

for $\Phi_2 \leq E_1 \leq \Phi_1$, and

$$\begin{aligned} T = {} & 4\sqrt{E_1(E_1 - \Phi_2)}(E_1 - \Phi_1) \\ & \times \Big[(E_1 - \Phi_1) \left(2E_1 - \Phi_2 + 2\sqrt{E_1(E_1 - \Phi_2)} \right) \\ & + \Phi_1(\Phi_1 - \Phi_2) \sin^2\left(\sqrt{2m(E_1 - \Phi_1)} L/\hbar \right) \Big]^{-1} \end{aligned}$$

for $E_1 \geq \Phi_1$. Classical mechanics, on the other hand predicts $T = 0$ for $E_1 < \Phi_1$ and $T = 1$ for $E_1 > \Phi_1$, in stark contrast to the quantum mechanical transmission coefficient shown in Figure 3.2.

The phenomenon that particles can tunnel through regions even when they do not have the required energy is denoted as *tunnel effect*. It has been observed in many instances in nature and technology, e.g. in the α decay of radioactive nuclei (Gamow, 1928) or electron tunneling in heavily doped pn junctions (Esaki, 1958). Esaki diodes actually provide a beautiful illustration of the interplay of two quantum effects, *viz.* energy bands in solids and tunneling. Charge carriers can tunnel from one energy band into a different energy band in heavily doped pn junctions. We will discuss energy bands in Chapter 10.

Quantum mechanical tunneling is also used e.g. in scanning tunneling microscopes (Binnig & Rohrer, 1982), and in flash memory and magnetic tunnel junction devices[4].

It is easy to understand from our results for the transmission probability why quantum mechanical tunneling plays such an important role in modern memory devices. If we want to have a memory device which is electrically controlled, then

[4]Magnetic tunnel junctions provide yet another beautiful example of the interplay of two quantum effects – tunneling and exchange interactions. Exchange interactions will be discussed in Chapter 17.

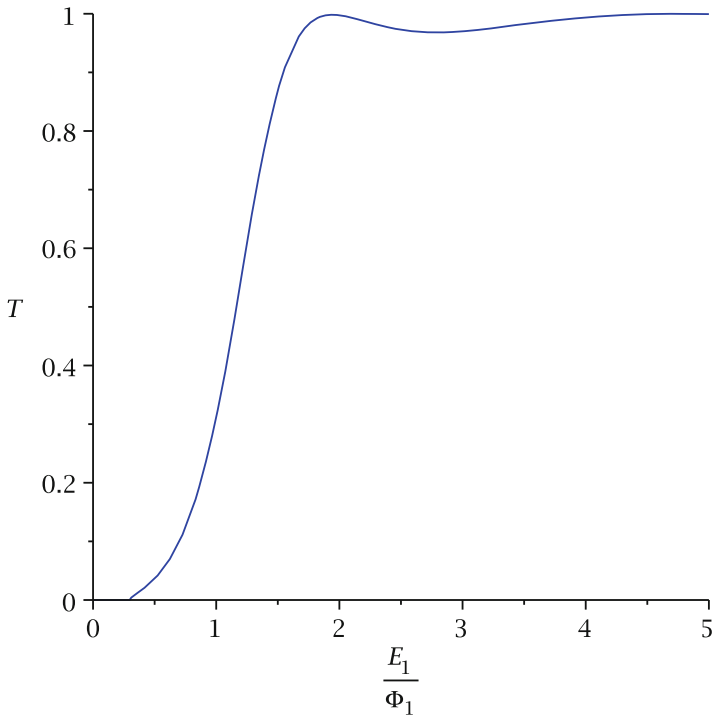

Fig. 3.2 The transmission coefficient for a non-symmetric square barrier. The curve calculated here corresponds to $m = 511\,\text{keV}/c^2$, $\Phi_1 = 10\,\text{eV}$, $\Phi_2 = 3\,\text{eV}$, $L = 2\,\text{Å}$

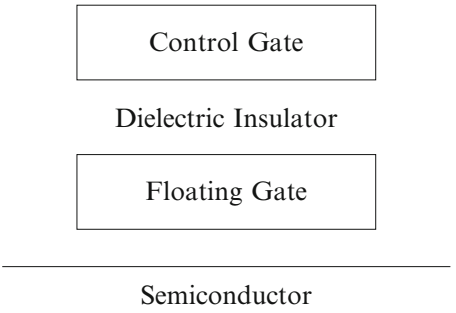

Fig. 3.3 A simplified schematic of a flash memory cell. The tunneling barrier is the thin section of the insulator between the floating gate and the semiconductor

apparently the information bits 0 and 1 can be encoded through the two states of a device being electrically charged or neutral. If we also want to maintain storage of the information even when the power supply is switched off (a *non-volatile memory*), then the device should not discharge spontaneously, i.e. it should be electrically insulated. The device should therefore be a conductor which is surrounded by insulating material. Such a device is called a *floating gate* in flash memory devices, see Figure 3.3.

However, we do want to be able to charge or discharge the floating gate, i.e. eventually we want to run a current through the surrounding insulator without destroying it. Using a tunneling current through the insulator is an elegant way to achieve this. Our results for the tunneling probability tell us how to switch a tunneling current. If we substitute $m = 511\ \mathrm{keV}/c^2$, $\Phi_1 - E_1 \simeq 1$ eV, and $L \simeq 10$ nm, we find

$$\sqrt{2m(\Phi_1 - E_1)}L/\hbar \simeq 51$$

and therefore

$$\sinh^2\Big(\sqrt{2m(\Phi_1 - E_1)}L/\hbar\Big) \simeq \frac{1}{4}\exp\Big(2\sqrt{2m(\Phi_1 - E_1)}L/\hbar\Big)\,,$$

i.e. in excellent approximation

$$T \simeq 16\frac{\sqrt{E_1(E_1 - \Phi_2)}(\Phi_1 - E_1)}{\Phi_1(\Phi_1 - \Phi_2)}\exp\Big(-2\sqrt{2m(\Phi_1 - E_1)}L/\hbar\Big)\,.$$

The exponential dependence on $\sqrt{\Phi_1 - E_1}$ implies that decreasing $\Phi_1 - E_1$ by increasing E_1 will have a huge impact on the tunneling current through the insulator. We can control the energy E_1 of the electrons in the floating gate through the electron concentration in a nearby control gate. Presence of a negative charge on the nearby control gate will increase the energy of any electrons stored in the floating gate and allow them to tunnel into a conducting sink (usually a semiconductor) opposite to the control gate. This process will discharge the floating gate. On the other hand, a positive charge on the control gate will attract electrons from an electron current through the semiconductor towards the insulating barrier and help them to tunnel into the floating gate.

3.2 Box approximations for quantum wells, quantum wires and quantum dots

A particle in three dimensions which can move freely in two directions, but is confined in one direction, is said to be confined in a quantum well. A particle which can move freely only in one direction but is confined in two directions is confined in a quantum wire. Finally, a particle which is confined to a small region of space is confined to a quantum dot. We will discuss energy levels and wave functions of particles in all three situations in the approximation of confinement to rectangular (box-like) regions. For the quantum well this means that our particle will be confined to the region $0 < x < L_1$, but it can move freely in y and z direction. The particle in the quantum wire is confined in x and y direction to $0 < x < L_1$, $0 < y < L_2$, but

it can move freely in the z direction. Finally, box approximation for a quantum dot means that the particle is confined to the box $0 < x < L_1$, $0 < y < L_2$, $0 < z < L_3$.

We will assume strict confinement in this section, i.e. the wave function of the particle vanishes outside of the allowed region while the wave function inside the region must continuously go to zero at the boundaries of the allowed region.

We gauge the energy axis such that in the allowed region the potential energy of the particle vanishes, $V(\boldsymbol{x}) = 0$, i.e. the time-independent three-dimensional Schrödinger equation in the allowed region takes the form

$$E\psi(\boldsymbol{x}) = -\frac{\hbar^2}{2m}\Delta\psi(\boldsymbol{x}). \tag{3.7}$$

Substitution of the Fourier decomposition

$$\psi(\boldsymbol{x}) = \frac{1}{\sqrt{2\pi}^3}\int d^3\boldsymbol{k}\,\psi(\boldsymbol{k})\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})$$

yields $k = \sqrt{2mE}/\hbar$ and the general solution for given energy E takes the form

$$\psi(\boldsymbol{x}) = \int d^2\hat{\boldsymbol{k}}\,A(\hat{\boldsymbol{k}})\exp\left(\frac{\mathrm{i}}{\hbar}\sqrt{2mE}\hat{\boldsymbol{k}}\cdot\boldsymbol{x}\right), \quad \hat{\boldsymbol{k}}^2 = 1.$$

On the other hand, equation (3.7) tells us that the energy of a plane wave $\psi(\boldsymbol{x}) = \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})/\sqrt{2\pi}^3$ of momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$ is

$$E = \frac{\hbar^2\boldsymbol{k}^2}{2m}. \tag{3.8}$$

If we have no confinement condition at all, our particle is a free particle and equation (3.8) is the kinetic energy of a free non-relativistic particle of momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$.

Energy levels in a quantum well

If we have a confinement condition in x-direction, e.g. $\psi(0, y, z) = 0$ and $\psi(L_1, y, z) = 0$, then we have to superimpose plane wave solutions in x direction to form a standing wave with nodes at the boundary points, and we find solutions

$$\psi_{n_1,k_2,k_3}(\boldsymbol{x}) = \frac{1}{\pi\sqrt{2L_1}}\exp[\mathrm{i}(k_2 y + k_3 z)]\sin\left(\frac{n_1\pi x}{L_1}\right), \tag{3.9}$$

with integer $n_1 \in \mathbb{N}$ and energy

$$E_{n_1,k_2,k_3} = \frac{\hbar^2}{2m}\left(k_2^2 + k_3^2 + \frac{n_1^2\pi^2}{L_1^2}\right).$$

The energy of the particle is therefore determined by the discrete quantum number n_1 and the continuous wave numbers k_2 and k_3.

Energy levels in a quantum wire

If the particle is confined both in the x-direction to the region $0 < x < L_1$ and in the y-direction to the region $0 < y < L_2$, the boundary conditions $\psi(0, y, z) = 0$, $\psi(L_1, y, z) = 0$, $\psi(x, 0, z) = 0$ and $\psi(x, L_2, z) = 0$ yield

$$\psi_{n_1,n_2,k_3}(\boldsymbol{x}) = \sqrt{\frac{2}{\pi L_1 L_2}}\exp(\mathrm{i}k_3 z)\sin\left(\frac{n_1\pi x}{L_1}\right)\sin\left(\frac{n_2\pi x}{L_2}\right), \tag{3.10}$$

and the energy of the particle is determined by the discrete quantum numbers n_1 and n_2 and the continuous wave number k_3 for motion in z direction,

$$E_{n_1,n_2,k_3} = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2}\right) + \frac{\hbar^2 k_3^2}{2m}.$$

Energy levels in a quantum dot

If the particle is confined to the region $0 < x < L_1$, $0 < y < L_2$, $0 < z < L_3$, the conditions of vanishing wave function on the boundaries yields normalized states

$$\psi_{n_1,n_2,n_3}(\boldsymbol{x}) = \sqrt{\frac{8}{L_1 L_2 L_3}}\sin\left(\frac{n_1\pi x}{L_1}\right)\sin\left(\frac{n_2\pi y}{L_2}\right)\sin\left(\frac{n_3\pi z}{L_3}\right), \tag{3.11}$$

and the energy levels are determined in terms of three discrete quantum numbers,

$$E_{n_1,n_2,n_3} = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2}\right). \tag{3.12}$$

Degeneracy of quantum states

If two or more different quantum states have the same energy, the quantum states are said to be degenerate, and the corresponding energy level is also denoted as degenerate. This happens e.g. for the quantum wire and the quantum dot if at least

two of the length scales L_i have the same value. We will discuss the quantum dot (3.12, 3.11) with $L_1 = L_2 = L_3 \equiv L$ as an example. This cubic quantum dot has energy levels

$$E_{n_1,n_2,n_3} = \left(n_1^2 + n_2^2 + n_3^2\right) \frac{\pi^2\hbar^2}{2mL^2}.$$

The lowest energy level

$$E_{1,1,1} = 3\frac{\pi^2\hbar^2}{2mL^2}$$

corresponds to a unique quantum state $\psi_{1,1,1}(\boldsymbol{x})$ and is therefore not degenerate. However, the next allowed energy value

$$E_{1,1,2} = E_{1,2,1} = E_{2,1,1} = 6\frac{\pi^2\hbar^2}{2mL^2}$$

is realized for three different wave functions $\psi_{1,1,2}(\boldsymbol{x})$, $\psi_{1,2,1}(\boldsymbol{x})$ and $\psi_{2,1,1}(\boldsymbol{x})$, and is therefore *three-fold degenerate*. Three-fold degeneracy is also realized for the next two energy levels

$$E_{1,2,2} = E_{2,1,2} = E_{2,2,1} = 9\frac{\pi^2\hbar^2}{2mL^2}$$

and

$$E_{1,1,3} = E_{1,3,1} = E_{3,1,1} = 11\frac{\pi^2\hbar^2}{2mL^2}.$$

The next energy level is again non-degenerate,

$$E_{2,2,2} = 12\frac{\pi^2\hbar^2}{2mL^2}.$$

Then follows a six-fold degenerate energy level,

$$E_{1,2,3} = E_{2,3,1} = E_{3,1,2} = E_{1,3,2} = E_{3,2,1} = E_{2,1,3} = 14\frac{\pi^2\hbar^2}{2mL^2}.$$

3.3 The attractive δ function potential

The attractive δ function potential

$$V(x) = -\mathcal{W}\delta(x), \quad \mathcal{W} > 0,$$

provides a simple model system for co-existence of free states and bound states of particles in a potential.

Positive energy solutions of the stationary Schrödinger equation for the δ function potential must have the form

$$\psi_k(x) = \sum_{\pm} \Theta(\pm x)\left[A_\pm \exp(\mathrm{i}kx) + B_\pm \exp(-\mathrm{i}kx)\right], \quad \hbar k = \sqrt{2mE},$$

and normalizability limits the negative energy solutions to the from

$$\psi_\kappa(x) = \sum_{\pm} \Theta(\pm x) C_\pm \exp(\mp\kappa x), \quad \hbar\kappa = \sqrt{-2mE}.$$

These solutions must be continuous in order not to generate $\delta'(x)$ terms which would violate the Schrödinger equation,

$$A_+ + B_+ = A_- + B_-, \quad C_+ = C_-. \tag{3.13}$$

On the other hand, integrating the Schrödinger equation from $x = -\epsilon$ to $x = \epsilon$ and taking the limit $\epsilon \to 0+$ yields the junction conditions

$$\lim_{\epsilon\to 0+}\left(\left.\frac{d\psi(x)}{dx}\right|_{x=\epsilon} - \left.\frac{d\psi(x)}{dx}\right|_{x=-\epsilon}\right) = -\frac{2m}{\hbar^2}\mathcal{W}\psi(0).$$

This implies

$$\mathrm{i}k(A_+ - B_+ - A_- + B_-) = -\frac{m}{\hbar^2}\mathcal{W}(A_+ + B_+ + A_- + B_-) \tag{3.14}$$

for the free states and

$$\kappa = \frac{m}{\hbar^2}\mathcal{W} \tag{3.15}$$

for the bound states.

Equation (3.15) tells us that there exists one bound state for $\mathcal{W} > 0$ with energy

$$E_\kappa = -\frac{m}{2\hbar^2}\mathcal{W}^2.$$

The normalized bound state is

$$\psi_\kappa(x) = \sqrt{\kappa}\exp(-\kappa|x|). \tag{3.16}$$

For the free states, we first look at solutions which are right or left moving plane waves $\exp(\pm\mathrm{i}kx)/\sqrt{2\pi}$ on the half-line $x > 0$, i.e. we solve equations (3.13) and (3.14) first under the conditions $A_+ = 1/\sqrt{2\pi}$, $B_+ = 0$, and then under the conditions $A_+ = 0$, $B_+ = 1/\sqrt{2\pi}$. This yields solutions

$$\psi_{+k}(x) = \frac{1}{\sqrt{2\pi}} \exp(\mathrm{i}kx) + \sqrt{\frac{2}{\pi}}\Theta(-x)\frac{\kappa}{k}\sin(kx), \tag{3.17}$$

$$\psi_{-k}(x) = \frac{1}{\sqrt{2\pi}} \exp(-\mathrm{i}kx) + \sqrt{\frac{2}{\pi}}\Theta(-x)\frac{\kappa}{k}\sin(kx).$$

The free solutions can be unified if we also allow for negative values of k (recall that until now k was defined positive from $\hbar k = \sqrt{2mE}$),

$$\psi_k(x) = \frac{1}{\sqrt{2\pi}} \exp(\mathrm{i}kx) + \sqrt{\frac{2}{\pi}}\Theta(-x)\frac{\kappa}{k}\sin(kx). \tag{3.18}$$

These states are free right or left moving plane waves for $x > 0$, but they do not provide orthonormal bases for the scattering states in the attractive δ potential. We will construct two orthonormal bases below in (3.21, 3.22) and (3.25, 3.26), respectively.

Another useful representation for the free states is motivated by considering the outgoing waves with amplitudes A_+ and B_- as consequences of the incident waves with amplitudes A_- and B_+. The junction conditions (3.13, 3.14) yield

$$\begin{pmatrix} A_+ \\ B_- \end{pmatrix} = \frac{1}{k - \mathrm{i}\kappa} \begin{pmatrix} k & \mathrm{i}\kappa \\ \mathrm{i}\kappa & k \end{pmatrix} \cdot \begin{pmatrix} A_- \\ B_+ \end{pmatrix}. \tag{3.19}$$

The unitary matrix

$$\underline{S} = \frac{1}{k - \mathrm{i}\kappa} \begin{pmatrix} k & \mathrm{i}\kappa \\ \mathrm{i}\kappa & k \end{pmatrix} = \frac{1}{\sqrt{E} - \mathrm{i}\sqrt{B}} \begin{pmatrix} \sqrt{E} & \mathrm{i}\sqrt{B} \\ \mathrm{i}\sqrt{B} & \sqrt{E} \end{pmatrix} \tag{3.20}$$

is also known as a *scattering matrix* because it describes scattering of incoming waves off the potential. Here $B \equiv -E_\kappa$ is the binding energy of the bound state.

The scattering matrix can be used to read off the reflection and transmission coefficients for the δ function potential,

$$R = \left|\frac{\partial B_-}{\partial A_-}\right|^2 = \left|\frac{\partial A_+}{\partial B_+}\right|^2 = \frac{\kappa^2}{k^2 + \kappa^2} = \frac{B}{E + B},$$

$$T = \left|\frac{\partial A_+}{\partial A_-}\right|^2 = \left|\frac{\partial B_-}{\partial B_+}\right|^2 = \frac{k^2}{k^2 + \kappa^2} = \frac{E}{E + B}.$$

In many situations it is also convenient to use even and odd solutions of the Schrödinger equation. Odd (or *negative parity*) solutions $\psi(x) = -\psi(-x)$ must satisfy $A_+ = -B_-$, $B_+ = -A_-$. Solving equations (3.13) and (3.14) with these conditions yields the negative parity solutions

$$\psi_{k,-}(x) = \frac{1}{\sqrt{\pi}}\sin(kx). \tag{3.21}$$

The positive energy solutions of positive parity follow from $A_+ = B_-$, $B_+ = A_-$ and equations (3.13), (3.14) in the form

$$\psi_{k,+}(x) = \frac{1}{\sqrt{\pi}} \frac{k\cos(kx) - \kappa\,\sin(k|x|)}{\sqrt{\kappa^2 + k^2}}. \tag{3.22}$$

The wave number k in (3.21) and (3.22) is constrained to the positive half-line $k = \sqrt{2mE}/\hbar > 0$.

The solutions (3.16), (3.21) and (3.22) satisfy the usual orthonormalization conditions for bound or free states, respectively (see Problem 3.9), and their completeness relation is

$$\psi_\kappa(x)\psi_\kappa(x') + \int_0^\infty dk \left[\psi_{k,-}(x)\psi_{k,-}(x') + \psi_{k,+}(x)\psi_{k,+}(x')\right] = \delta(x-x'). \tag{3.23}$$

The state (3.17) describes a situation in which a particle is incident on the δ potential from the left, and therefore on the right side of the potential ($x > 0$) we only have the right moving transmitted component, whereas the wave function for $x < 0$ contains both incoming and reflected components. We can find a corresponding normalized solution and construct a basis of scattering states which describe scattering of particles incident from the left or from the right by applying a unitary transformation on the basis of even and odd scattering states (3.22, 3.21):

$$\begin{pmatrix} \psi_{k,l}(x) \\ \psi_{k,r}(x) \end{pmatrix} = \frac{1}{\sqrt{2(\kappa^2 + k^2)}} \begin{pmatrix} \sqrt{\kappa^2 + k^2} & \kappa + \mathrm{i}k \\ \sqrt{\kappa^2 + k^2} & -\kappa - \mathrm{i}k \end{pmatrix} \begin{pmatrix} \psi_{k,+}(x) \\ \psi_{k,-}(x) \end{pmatrix}. \tag{3.24}$$

This yields a basis with states describing incidence of particles from the left,

$$\psi_{k,l}(x) = \frac{k\exp(\mathrm{i}kx) + 2\kappa\Theta(-x)\sin(kx)}{\sqrt{2\pi(\kappa^2 + k^2)}}, \tag{3.25}$$

and incidence of particles from the right,

$$\psi_{k,r}(x) = \frac{k\exp(-\mathrm{i}kx) - 2\kappa\Theta(x)\sin(kx)}{\sqrt{2\pi(\kappa^2 + k^2)}}. \tag{3.26}$$

The completeness relation is

$$\psi_\kappa(x)\psi_\kappa(x') + \int_0^\infty dk \left[\psi_{k,l}(x)\psi_{k,l}(x') + \psi_{k,r}(x)\psi_{k,r}(x')\right] = \delta(x-x'). \tag{3.27}$$

There is no bound state solution for a repulsive δ potential

$$V(x) = \mathcal{W}\delta(x) = \frac{\hbar^2\kappa}{m}\delta(x)$$

and the even parity energy eigenstates become

$$\phi_{k,+}(x) = \frac{1}{\sqrt{\pi}} \frac{k\cos(kx) + \kappa \sin(k|x|)}{\sqrt{\kappa^2 + k^2}}. \tag{3.28}$$

The completeness relation for the eigenfunctions of the repulsive δ potential is therefore

$$\int_0^\infty dk \left[\psi_{k,-}(x)\psi_{k,-}(x') + \phi_{k,+}(x)\phi_{k,+}(x')\right] = \delta(x - x'). \tag{3.29}$$

3.4 Evolution of free Schrödinger wave packets

Another important model system for quantum behavior is provided by free wave packets. We will discuss in particular free Gaussian wave packets because they provide a simple analytic model for dispersion of free wave packets. This example will also demonstrate that the spatial and temporal range of free particle models is constrained in quantum physics. We will see that free wave packets of subatomic particles disperse on relatively short time scales, which are however too long to interfere with lab experiments involving free electrons or nucleons. Nevertheless, the discussion of the dispersion of free wave packets makes it also clear that simple interpretations of particles in quantum mechanics as highly localized free wave packets which every now and then get disturbed through interactions with other wave packets are not feasible. Particles can exist in the form of not too small free wave packets for a little while, but atomic or nuclear size wave packets must be stabilized by interactions to avoid rapid dispersion. We will see examples of stable wave packets in Chapters 6 and 7.

The free Schrödinger propagator

Substitution of a Fourier *ansatz*

$$\psi(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} d\omega\, \psi(k,\omega) \exp[\mathrm{i}(kx - \omega t)]$$

into the free Schrödinger equation shows that the general solution of that equation in one dimension is given in terms of a wave packet

$$\psi(k,\omega) = \sqrt{2\pi}\psi(k)\delta\left(\omega - \frac{\hbar k^2}{2m}\right),$$

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \psi(k) \exp\left[\mathrm{i}\left(kx - \frac{\hbar k^2}{2m}t\right)\right]. \tag{3.30}$$

The amplitude $\psi(k)$ is related to the initial condition $\psi(x,0)$ through inverse Fourier transformation

$$\psi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \psi(x,0) \exp(-\mathrm{i}kx)\,,$$

and substitution of $\psi(k)$ into (3.30) leads to the expression

$$\psi(x,t) = \int_{-\infty}^{\infty} dx'\, U(x-x',t)\psi(x',0) \tag{3.31}$$

with the free *propagator*

$$U(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, \exp\left[\mathrm{i}\left(kx - \frac{\hbar k^2}{2m}t\right)\right]. \tag{3.32}$$

This is sometimes formally integrated as[5]

$$U(x,t) = \sqrt{\frac{m}{2\pi\mathrm{i}\hbar t}} \exp\left(\mathrm{i}\frac{mx^2}{2\hbar t}\right). \tag{3.33}$$

The propagator is the particular solution of the free Schrödinger equation

$$\mathrm{i}\hbar \frac{\partial}{\partial t} U(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} U(x,t)$$

with initial condition $U(x,0) = \delta(x)$. It yields the corresponding *retarded Green's function*

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \mathcal{G}(x,t) + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \mathcal{G}(x,t) = \delta(t)\delta(x), \tag{3.34}$$

$$\mathcal{G}(x,t)\Big|_{t<0} = 0, \tag{3.35}$$

through

$$\mathcal{G}(x,t) = \frac{\Theta(t)}{\mathrm{i}\hbar} U(x,t). \tag{3.36}$$

This can also be derived from the Fourier decomposition of equation (3.34), which yields

[5]The propagator is commonly denoted as $K(x,t)$. However, we prefer the notation $U(x,t)$ because the propagator is nothing but the x representation of the time evolution operator $U(t)$ introduced in Chapter 13.

$$\mathcal{G}(x,t) = \frac{1}{(2\pi)^2\hbar}\int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} d\omega\, \frac{\exp[\mathrm{i}(kx-\omega t)]}{\omega - (\hbar k^2/2m) + \mathrm{i}\epsilon}.$$

The negative imaginary shift of the pole $(\hbar k^2/2m) - \mathrm{i}\epsilon$, $\epsilon \to +0$, in the complex ω plane ensures that the condition (3.35) is satisfied. We will encounter time evolution operators and Green's functions in many places in this book. The designation *propagator* is often used both for the time evolution operator $U(x,t)$ and for the related Green's function $\mathcal{G}(x,t)$. $U(x,t)$ propagates initial conditions as in equation (3.31) while $\mathcal{G}(x,t)$ propagates perturbations or source terms in the Schrödinger equation.

Width of Gaussian wave packets

A wave packet $\psi(x,t)$ is denoted as a *Gaussian wave packet* if $|\psi(x,t)|^2$ is a Gaussian function of x. We will see below through direct Fourier transformation that $\psi(x,t)$ is a Gaussian wave packet in x if and only if $\psi(k,t)$ is a Gaussian wave packet in k.

Normalized Gaussian wave packets have the general form

$$\psi(x,t) = \left(\frac{2\alpha(t)}{\pi}\right)^{\frac{1}{4}} \exp\bigl(-\alpha(t)[x-x_0(t)]^2 + \mathrm{i}\varphi(x,t)\bigr)\,, \tag{3.37}$$

and we will verify that the real coefficient $\alpha(t)$ is related to the variance through $\Delta x^2(t) = 1/4\alpha(t)$. The expectation values of x and x^2 are readily evaluated,

$$\begin{aligned}\langle x\rangle(t) &= \sqrt{\frac{2\alpha(t)}{\pi}}\int_{-\infty}^{\infty} dx\, x \exp\bigl(-2\alpha(t)[x-x_0(t)]^2\bigr)\\ &= \sqrt{\frac{2\alpha(t)}{\pi}}\int_{-\infty}^{\infty} d\xi\, [\xi + x_0(t)] \exp\bigl(-2\alpha(t)\xi^2\bigr) = x_0(t),\end{aligned}$$

$$\begin{aligned}\langle x^2\rangle(t) &= \sqrt{\frac{2\alpha(t)}{\pi}}\int_{-\infty}^{\infty} dx\, x^2 \exp\bigl(-2\alpha(t)[x-x_0(t)]^2\bigr)\\ &= \sqrt{\frac{2\alpha(t)}{\pi}}\int_{-\infty}^{\infty} d\xi\, [\xi + x_0(t)]^2 \exp\bigl(-2\alpha(t)\xi^2\bigr)\\ &= \sqrt{\frac{2\alpha(t)}{\pi}}\left(x_0^2(t) - \frac{1}{2}\frac{d}{d\alpha(t)}\right)\int_{-\infty}^{\infty} d\xi\, \exp\bigl(-2\alpha(t)\xi^2\bigr)\\ &= x_0^2(t) + \frac{1}{4\alpha(t)},\end{aligned}$$

and therefore we find indeed

$$\Delta x^2(t) = \langle x^2\rangle(t) - \langle x\rangle^2(t) = \frac{1}{4\alpha(t)}. \tag{3.38}$$

Free Gaussian wave packets in Schrödinger theory

We assume that the wave packet of a free particle at time $t = 0$ was a Gaussian wave packet of width Δx,

$$\psi(x,0) = \frac{1}{(2\pi\Delta x^2)^{1/4}} \exp\left(-\frac{(x-x_0)^2}{4\Delta x^2} + \mathrm{i}k_0 x\right). \tag{3.39}$$

This yields a Gaussian wave packet of constant width

$$\Delta k = \frac{1}{2\Delta x}$$

in k space,

$$\begin{aligned}
\psi(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \psi(x,0) \exp(-\mathrm{i}kx) \\
&= \frac{1}{(2\pi)^{3/4}(\Delta x^2)^{1/4}} \int_{-\infty}^{\infty} dx\, \exp\left(-\frac{(x-x_0)^2}{4\Delta x^2} + \mathrm{i}(k_0-k)x\right) \\
&= \frac{\exp[\mathrm{i}(k_0-k)x_0]}{(2\pi)^{3/4}(\Delta x^2)^{1/4}} \int_{-\infty}^{\infty} d\xi\, \exp\left[-\frac{\xi^2}{4\Delta x^2} + \mathrm{i}(k_0-k)\xi\right] \\
&= \left(\frac{2\Delta x^2}{\pi}\right)^{\frac{1}{4}} \exp\left[-\Delta x^2(k-k_0)^2 - \mathrm{i}(k-k_0)x_0\right],
\end{aligned} \tag{3.40}$$

$$\psi(k,t) = \psi(k) \exp\left(-\mathrm{i}\frac{\hbar k^2}{2m}t\right). \tag{3.41}$$

Substitution of $\psi(k)$ into equation (3.30) then yields

$$\begin{aligned}
\psi(x,t) &= \left(\frac{\Delta x^2}{2\pi^3}\right)^{\frac{1}{4}} \exp\left(-\Delta x^2 k_0^2 + \mathrm{i}k_0 x_0\right) \\
&\quad \times \int_{-\infty}^{\infty} dk\, \exp\left[-\left(\Delta x^2 + \mathrm{i}\frac{\hbar t}{2m}\right)k^2 + \left(2\Delta x^2 k_0 + \mathrm{i}(x-x_0)\right)k\right] \\
&= \frac{(2\pi\Delta x^2)^{1/4}}{[2\pi\Delta x^2 + \mathrm{i}\pi(\hbar t/m)]^{1/2}} \exp\left(-\Delta x^2 k_0^2 + \mathrm{i}k_0 x_0\right)
\end{aligned}$$

$$\times \exp\left[\frac{\left[2\Delta x^2 k_0 + \mathrm{i}(x - x_0)\right]^2}{4\Delta x^2 + 2\mathrm{i}(\hbar t/m)}\right]$$

$$= \frac{(2\pi\Delta x^2)^{1/4}}{[2\pi\Delta x^2 + \mathrm{i}\pi(\hbar t/m)]^{1/2}} \exp\left[-\frac{[x - x_0 - (\hbar k_0/m)t]^2}{4\Delta x^2 + (\hbar^2 t^2/m^2\Delta x^2)}\right]$$

$$\times \exp\left[\mathrm{i}\left(k_0 x - \frac{\hbar k_0^2}{2m}t + \frac{\hbar t}{8m}\frac{[x - x_0 - (\hbar k_0/m)t]^2}{(\Delta x^2)^2 + (\hbar^2 t^2/4m^2)}\right)\right]. \tag{3.42}$$

Comparison of equation (3.42) with equations (3.37, 3.38) yields

$$\Delta x^2(t) = \Delta x^2 + \frac{\hbar^2 t^2}{4m^2\Delta x^2}, \tag{3.43}$$

i.e. a strongly localized packet at time $t = 0$ will disperse very fast, because the dispersion time scale τ is proportional to Δx^2. The reason for the fast dispersion is that a strongly localized packet at $t = 0$ comprises many different wavelengths. However, each monochromatic component in a free wave packet travels with its own phase velocity

$$v(k) = \frac{\omega}{k} = \frac{\hbar k}{2m},$$

and a free strongly localized packet therefore had to emerge from rapid collapse and will disperse very fast. On the other hand, a poorly localized packet is almost monochromatic and therefore slowly changes in shape.

The relevant time scale for decay of the wave packet is

$$\tau = \frac{2m\Delta x^2}{\hbar}. \tag{3.44}$$

Electron guns often have apertures in the millimeter range. Assuming $\Delta x = 1\,\mathrm{mm}$ for an electron wave packet yields $\tau \simeq 2 \times 10^{-2}$ seconds. This sounds like a short time scale for dispersion of the wave packet. However, on the time scales of a typical lab experiment involving free electrons, dispersion of electron wave packets is completely negligible, see e.g. Problem 3.17.

On the other hand, suppose we can produce a free electron wave packet with atomic scale localization, $\Delta x = 1\,\text{Å}$. This wave packet would disperse with an extremely short time scale $\tau \simeq 2 \times 10^{-16}$ seconds, which means that the wave function of that electron would be smeared across the planet within a minute. See also Problem 3.18 for a corresponding discussion for neutrons.

We will see in Chapters 6 and 7 that wave packets can remain localized under the influence of forces, i.e. the notion of stable electrons in atoms makes sense, although the notion of highly localized *free* electrons governed by the *free* Schrödinger equation is limited to small distance and time scales.

We can infer from the example of the free Gaussian wave packet that the kinetic term in the Schrödinger equation drives wave packets apart. If there is no attractive potential term, the kinetic term decelerates any eventual initial contraction of a free wave packet and ultimately pushes the wave packet towards accelerated dispersion. We will see that this action of the kinetic term can be compensated by attractive potential terms in the Schrödinger equation. Balance between the collapsing force from attractive potentials and the dispersing force from the kinetic term can stabilize quantum systems.

Comparison of equation (3.41) with equations (3.37, 3.38) yields constant width of the wave packet in k space and therefore

$$\Delta p = \hbar \Delta k = \frac{\hbar}{2\Delta x},$$

i.e. there is no dispersion in momentum. The product of uncertainties of momentum and location of the particle satisfies $\Delta p \Delta x(t) \geq \hbar/2$, in agreement with Heisenberg's uncertainty relation, which will be derived for general wave packets in Section 5.1.

The energy expectation value and uncertainty of the wave packet are

$$\langle E \rangle = \frac{\hbar^2}{2m}\left(k_0^2 + \frac{1}{4\Delta x^2}\right)$$

and

$$\Delta E = \frac{\hbar^2}{2m}\sqrt{\frac{k_0^2}{\Delta x^2} + \frac{1}{8\Delta x^4}}.$$

Suppose we want to observe strong localization of a free particle. The decay time (3.44) then defines a measure for the time window Δt of observability of the particle. This satisfies

$$\Delta E \Delta t = \hbar\sqrt{\frac{1}{8} + k_0^2 \Delta x^2} \geq \frac{\hbar}{\sqrt{8}},$$

in agreement with the qualitative energy-time uncertainty relation (5.7), which we will encounter in Section 5.1.

The free Gaussian wave packet reproduces momentum eigenstates in the limit $\Delta x^2 \to \infty$ in the sense

$$\lim_{\Delta x^2 \to \infty}\left(\frac{\Delta x^2}{2\pi}\right)^{1/4} \psi(k) = \delta(k - k_0),$$

$$\lim_{\Delta x^2 \to \infty}\left(\frac{\Delta x^2}{2\pi}\right)^{1/4} \psi(x,t) = \frac{1}{\sqrt{2\pi}} \exp\left[\mathrm{i}\left(k_0 x - \frac{\hbar t}{2m}k_0^2\right)\right].$$

3.5 Problems

3.1. Show that the tunneling probability for the square barrier in Figure 3.1 always satisfies $T < 1$ if $\Phi_2 > 0$.

Remark. Don't be fooled by Figure 3.2. The first transmission maximum at $E_1 \simeq 2\Phi_1$ corresponds already to $T \simeq 0.998$ and the next transmission maximum is even closer to 1, but it only looks like the transmission probability would reach 1 in Figure 3.2.

Tunneling resonances $T = 1$ occur for $\Phi_2 = 0$. For which values of E_1 and k_1 do this tunneling resonances occur? Which geometric matching condition holds between the wavelength of the incident particles and the square barrier for the tunneling resonances?

3.2a. Calculate the reflection and transmission coefficients for a particle that falls down a potential step of height V_0.

3.2b. Calculate the reflection and transmission coefficients for a particle that runs against a potential step of height V_0 both for particle energy $0 < E < V_0$ and for $E > V_0$.

3.3. Calculate the reflection and transmission coefficients for a particle in the (x, y) plane which moves in the potential $V(x, y) = V_0\Theta(x)$. Assume that the particle initially approached the potential step from the left,

$$\psi_{in}(x, y) = A \exp[\mathrm{i}(k_x x + k_y y)], \quad x < 0, \quad k_x > 0.$$

Solution. The reflected wave function is

$$\psi_r(x, y) = B \exp[\mathrm{i}(-k_x x + k_y y)], \quad x < 0.$$

The time-independent Schrödinger equation for the transmitted component of the wave function

$$\psi_t(x, y) = C \exp[\mathrm{i}(k'_x x + k'_y y)], \quad x > 0,$$

implies

$$k_x^2 + k_y^2 = k_x'^2 + k_y'^2 + \frac{2mV_0}{\hbar^2}.$$

However, smoothness of the wave function across the step does not only have to hold for all times (this is what requires equal particle energy from equal time-dependence $\exp(-\mathrm{i}Et/\hbar)$ of the wave functions on both sides of the step), but also for all locations along the step, i.e. for all y values. The latter requirement implies

equal $\exp(ik_y y)$ factors on both sides of the step, and we find with $k'_y = k_y$ exactly the same set of conditions that apply to the one-dimensional step from Problem 2,

$$k_x^2 = k_x'^2 + \frac{2mV_0}{\hbar^2}, \quad A + B = C, \quad k_x(A - B) = k'_x C,$$

i.e. we find the same results as in Problem 2, except for the substitution $E \to E_x = \hbar^2 k_x^2/2m$ if we want to express results in terms of energies rather than wave numbers.

3.4. A barrier for motion of a particle consists of a combination of two repulsive δ function potentials with separation a,

$$V(x) = \mathcal{W}\delta(x) + \mathcal{W}\delta(x - a).$$

Calculate the reflection and transmission coefficients for particles with momentum $\hbar k$.

3.5. Why is there a simple relation between momentum uncertainty and energy level in the box model for a quantum dot? What is the relation?

3.6. A very simple cubic model for a color center in an alkali halide crystal consists of an electron confined to a cube of length L. How large is the length L if the electron absorbs photons of energy 2.3 eV?

Mollwo had found the empirical relation $\nu d^2 = 5.02 \times 10^{-5}\,\mathrm{m^2\,Hz}$ between absorption frequencies ν of color centers and lattice constants d in alkali halide crystals. For the simple cubic model, which relation between L and d follows from Mollwo's relation?

A spherical model is also very simple, but gives a better estimate for the ratio between size of the color center and lattice constant, see the corresponding problem in Chapter 7.

3.7. Calculate the momentum uncertainty in the bound state (3.16).

3.8. Calculate the scattering matrix for the square barrier from Section 3.1.

3.9. Show that the bound state (3.16) of the attractive δ potential is orthogonal to the free states (3.21, 3.22),

$$\int_{-\infty}^{\infty} dx\, \psi_{k,\pm}(x)\psi_\kappa(x) = 0.$$

Show also that the free eigenstates (3.21, 3.22) and (3.28) of the attractive or repulsive δ potential are normalized according to

$$\int_{-\infty}^{\infty} dx\, \psi_{k,-}(x)\psi_{k',-}(x) = \delta(k - k'), \quad \int_{-\infty}^{\infty} dx\, \psi_{k,+}(x)\psi_{k',+}(x) = \delta(k - k'),$$

$$\int_{-\infty}^{\infty} dx\, \phi_{k,+}(x)\phi_{k',+}(x) = \delta(k - k').$$

Remark. You have to use that the wave numbers k and k' are positive.

3.10. Construct a basis of scattering states for the repulsive δ potential which consists of states describing incidence of particles from the left or from the right on the potential.

3.11. Show that all the momentum expectation values $\langle p^n \rangle$ are conserved for a free particle.

If the particle is moving in a potential $V(x)$, find a necessary and sufficient condition for $V(x)$ such that $\langle p^n \rangle$ is constant.

3.12. Suppose $\psi(x,t)$ is a normalizable free wave packet in one dimension, e.g. the Gaussian wave packet from Section 3.4. Which classical quantity of the particle corresponds to the integral $\int dx\, j(x)$ of the current density? Does a similar result hold for $\int d^3\boldsymbol{x}\, \boldsymbol{j}(\boldsymbol{x})$ in three dimensions?

3.13. The wave function of a free particle at time $t = 0$ is

$$\psi(x,0) = \sqrt{\frac{2a^3}{\pi}}\,\frac{1}{x^2 + a^2}.$$

How large are the uncertainties $\Delta x(t)$ and Δp in location and momentum of the particle?

Remark. The wave function $\psi(x,t)$ of the particle can be expressed in terms of complex error functions, but it is easier to use the wave function $\psi(k,t)$ in k space for the calculation of the uncertainties.

3.14. The wave function of a free particle at time $t = 0$ is

$$\psi(x,0) = \sqrt{\kappa}\,\exp(-\kappa|x|)\,. \tag{3.45}$$

One could produce this state as initial state of a free particle by first capturing the particle in the bound state of an attractive δ potential and then switching off the potential.

Calculate the wave function $\psi(k,t)$ of the particle.

How large are the uncertainties $\Delta x(t)$ and Δp in location and momentum of the particle?

3.15. The wave function of a free particle at time $t = 0$ is

$$\begin{aligned}\psi(x,0) &= \frac{\Theta(x+a)\Theta(a-x)}{\sqrt{2a}} = \frac{\Theta(a-x) - \Theta(-x-a)}{\sqrt{2a}} \\ &= \frac{\Theta(x+a) - \Theta(x-a)}{\sqrt{2a}}.\end{aligned} \tag{3.46}$$

Calculate the wave function $\psi(x,t)$ of the particle.

Solution. The wave function in momentum space is

$$\psi(k) = \frac{1}{2\sqrt{\pi a}} \int_{-a}^{a} dx\, \exp(-\mathrm{i}kx) = \frac{\sin(ka)}{\sqrt{\pi a}k},$$

$$\psi(k,t) = \psi(k) \exp\left(-\mathrm{i}\frac{\hbar k^2}{2m}t\right).$$

The wave function $\psi(x,t)$ can be evaluated numerically from the first line of the following representations,

$$\begin{aligned}\psi(x,t) &= \frac{1}{2\pi\mathrm{i}\sqrt{2a}} \int_{-\infty}^{\infty} dk\, \frac{\exp[\mathrm{i}k(x+a)] - \exp[\mathrm{i}k(x-a)]}{k} \exp\left(-\mathrm{i}\frac{\hbar t}{2m}k^2\right) \\ &= \frac{1}{2\pi\mathrm{i}\sqrt{2a}} \int_{-\infty}^{\infty} dk\, \frac{\exp[\mathrm{i}k(x+a)] - \exp[\mathrm{i}k(x-a)]}{k+\mathrm{i}\epsilon} \exp\left(-\mathrm{i}\frac{\hbar t}{2m}k^2\right) \\ &= \frac{1}{2\pi\mathrm{i}\sqrt{2a}} \int_{-\infty}^{\infty} dk\, \frac{\exp[\mathrm{i}k(x+a)] - \exp[\mathrm{i}k(x-a)]}{k-\mathrm{i}\epsilon} \exp\left(-\mathrm{i}\frac{\hbar t}{2m}k^2\right).\end{aligned}$$

However, we can also proceed with the analytical evaluation of the integrals by using the observation

$$\pm\frac{\partial}{\partial a} \int_{-\infty}^{\infty} dk\, \frac{\exp[\mathrm{i}k(x\pm a)]}{k} \exp\left(-\mathrm{i}\frac{\hbar t}{2m}k^2\right) = \mathrm{i}\sqrt{\frac{2\pi m}{\mathrm{i}\hbar t}} \exp\left(\mathrm{i}\frac{m}{2\hbar t}(x\pm a)^2\right).$$

Integration with respect to the parameter a then yields

$$\psi(x,t) = \frac{1}{2\sqrt{2a}} \left[\mathrm{erf}\left(\sqrt{\frac{m}{2\mathrm{i}\hbar t}}(x+a)\right) - \mathrm{erf}\left(\sqrt{\frac{m}{2\mathrm{i}\hbar t}}(x-a)\right)\right], \tag{3.47}$$

where the error function is defined as

$$\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z du\, \exp(-u^2).$$

One can easily check that the error functions $\mathrm{erf}[\sqrt{m/2\mathrm{i}\hbar t}(x-x_0)]$ satisfy the free Schrödinger equation. The wave function $\psi(x,t)$ from equation (3.47) also satisfies the initial condition (3.46) through

$$\lim_{t\to 0-\mathrm{i}\epsilon} \mathrm{erf}\left(\sqrt{\frac{m}{2\mathrm{i}\hbar t}}(x-x_0)\right) = \Theta(x-x_0) - \Theta(x_0-x).$$

3.16. The initial condition (3.39) yielded a Gaussian wave packet that had its minimal spread in location x exactly at the time $t = 0$. Before that particular moment, the wave packet was contracting and afterwards it was spreading.

Find an initial condition $\psi(x, 0)$ for a Gaussian wave packet that will continue to contract for some time Δt before it expands.

3.17. In their famous verification of the wave properties of electrons through diffraction off the surface of a nickel crystal, Davisson and Germer[6] used an electron gun with an aperture of about 1 mm. The electron beam that produced the most prominent diffraction pattern had a kinetic energy of 54 eV, and the distance from the electron gun to the nickel target was 7 mm. Show that dispersion of the electron wave packet on the way from the electron gun to the target is completely negligible.

3.18. Suppose we could produce a free neutron with a nuclear scale width $\Delta x = 1$ fm. How large is the dispersion time scale (3.44) for the neutron?

Neutron beam experiments to measure e.g. the β decay of free neutrons use beams with apertures of a few centimeters[7]. How large is the dispersion time scale for neutrons with $\Delta x \simeq 3$ cm? How does this compare to the lifetime of free neutrons?

[6] C. Davisson, L.H. Germer, Phys. Rev. 30, 705 (1927).

[7] See e.g. J.M. Robson, Phys. Rev. 83, 349 (1951) for one of the early lifetime measurements of free neutrons, or H.P. Mumm *et al.*, Rev. Sci. Instrum. 75, 5343 (2004), for a modern experimental setup.