Chapter 2

Wave Mechanics and the Schrödinger equation

> *Falls es bei dieser verdammten Quantenspringerei bleiben sollte, so bedauere ich, mich jemals mit der Quantentheorie beschäftigt zu haben!*
> *-Erwin Schrödinger*

In this chapter we introduce the Schrödinger equation and its probabilistic interpretation. We then discuss some basic physical phenomena like wave packets, discrete bound state energies and scattering on the basis of one-dimensional examples.

2.1 The Schrödinger equation

Schrödingers wave mechanics originates in the work of Louis de Broglie on matter waves. De Broglie postulated that all material particles can have corpuscular as well as wavelike aspects and that the correspondence between the dynamical variables of the particle and the characteristic quantities of the associated wave,

$$E = \hbar\omega, \qquad \text{and} \qquad \vec{p} = \hbar\vec{k}, \tag{2.1}$$

which was established for photons by the Compton effect, continues to hold for all *matter waves*. Schrödinger extended these ideas and suggested that the dynamical state of a quantum system is completely described by a wave function ψ satisfying a homogeneous linear differential equation (so that different solutions can be superimposed, which is a typical property of waves). In particular, we can express ψ as a continuous superposition of plane waves,

$$\psi(\vec{x},t) = \int d^3k \; f(\vec{k})\, e^{i(\vec{k}\vec{x}-\omega(k)t)}. \tag{2.2}$$

For the plane waves $e^{i(\vec{k}\vec{x}-\omega t)}$ the relation (2.1) suggests the correspondence rule

$$\boxed{E \to i\hbar\frac{\partial}{\partial t}, \qquad \vec{p} \to \frac{\hbar}{i}\vec{\nabla}.} \tag{2.3}$$

Energy and momentum of a free classical particle are related by $E = p^2/2m$. When a particle moves in a potential $V(x)$ its conserved energy is given by the Hamilton function $H(x,p) = \frac{p^2}{2m} + V(x)$. Setting $E\psi = H\psi$ with $E \to i\hbar\partial_t$ and $\vec{p} \to \frac{\hbar}{i}\vec{\nabla}$ we arrive at the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t) \qquad \text{with} \qquad H = -\frac{\hbar^2}{2m}\Delta + V(x), \tag{2.4}$$

where $\Delta = \vec{\nabla}^2$ is the Laplace operator and $V = e\phi$ for an electron moving in an electric field $\vec{E}(x) = -\operatorname{grad}\phi(x)$.

More generally, a classical point particle with mass m and charge e moving in an electromagnetic field

$$\vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\partial_t\vec{A}, \qquad \vec{B} = \vec{\nabla}\times\vec{A} \tag{2.5}$$

with gauge potential $A^\mu = (\phi, \vec{A})$ feels a Lorentz force $\vec{F} = e(\vec{E} + \frac{1}{c}\vec{v}\times\vec{B})$. The Hamilton function describing this dynamics is[1]

$$H(x,p;t) = \frac{1}{2m}(\vec{p} - \frac{e}{c}\vec{A}(\vec{x},t))^2 + e\phi(\vec{x},t). \tag{2.6}$$

With the correspondence rule (2.3) we thus find the general Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2 + e\phi\right]\psi, \tag{2.7}$$

which describes the motion of a quantum mechanical scalar point particle in a classical external electromagnetic field. This is an approximation in several respects. First we have neglected the spin of elementary point particles like electrons, which we will discuss in chapter 5. In chapter 7 we will discuss the Dirac equation, which is the relativistic generalization of the Schrödinger equation. The relativistic treatment is necessary for a proper understanding of the magnetic interactions, and hence of the fine structure of the energy levels of hydrogen, and it will lead to the prediction of anti-matter. Eventually we should note that also the environment, including the electromagnetic field, consists of quantum systems. This leads to the "second quantization" of quantum field theory. First, however, we restrict our attention to the quantum mechanical description of a single non-relativistic point particle in a classical environment.

It is an important and surprising property of the Schrödinger equation that it explicitly depends on the electromagnetic potentials A^μ, which are unobservable and whose values depend on the coice of a gauge. This is in contrast to classical physics, where the Lorentz force is a

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[1] In order to derive the Lorentz force from this Hamiltonian we consider the canonical equations of motion

$$\dot{x}_i = \frac{\partial H}{\partial p_i} = \frac{p_i - \frac{e}{c}A_i}{m}, \qquad \dot{p}_j = -\frac{\partial H}{\partial x_j} = \frac{e}{c}\frac{\partial A_i}{\partial x_j}\frac{p_i - \frac{e}{c}A_i}{m} - e\frac{\partial\phi}{\partial x_j} = \frac{e}{c}(\partial_j A_i)\dot{x}_i - e\partial_j\phi,$$

which imply $\vec{F} = m\ddot{\vec{x}} = \frac{d}{dt}(p_i - \frac{e}{c}A_i) = \dot{\vec{p}} - \frac{e}{c}(\partial_t + \dot{x}_i\partial_i)\vec{A} = \frac{e}{c}(v_i\vec{\nabla}A_i - v_i\partial_i\vec{A}) - e(\frac{1}{c}\dot{\vec{A}} + \vec{\nabla}\phi) = \frac{e}{c}\vec{v}\times\vec{B} + e\vec{E}$. Note that the relation between the *canonical* momentum $p_j = m\dot{x}_j + \frac{e}{c}A_j$ and the velocity $\vec{v} = \dot{\vec{x}}$ depends on the gauge-dependent vector potential $\vec{A}$. The gauge-independent quantity $\vec{\pi} = m\dot{\vec{x}} = \vec{p} - \frac{e}{c}\vec{A}$ is sometimes called *physical* or *mechanical* momentum. According to the general quantization rule (see below) the operator $\frac{\hbar}{i}\vec{\nabla}$ has to replace the *canonical* momentum.

function of the gauge invariant field strengths. A straightforward calculation shows that a gauge transformation

$$\phi \to \phi' = \phi - \frac{1}{c}\frac{\partial}{\partial t}\Lambda, \qquad A \to A' = A + \vec{\partial}\Lambda \tag{2.8}$$

of the scalar and vector potentials, which leaves the observable fields $\vec{E}$ and $\vec{B}$ invariant for an arbitrary function $\Lambda(t, \vec{x})$, can be compensated by an space- and time-dependent phase rotation of the wave function[2]

$$\psi \to \psi' = e^{\frac{ie}{\hbar c}\Lambda}\psi, \tag{2.9}$$

i.e. if ψ solves the Schrödinger equation (2.7) then ψ' solves the same equation for potentials ϕ' and $\vec{A}'$. Since the phase of the wave function ψ can be changed arbitrarily by such a gauge transformation we might expect that only its modulus $|\psi(t, x)|$ is observable. This conclusion is indeed consistent with the physical interpretation of the wave function that was suggested by Max Born in 1927: $|\psi|^2(x) = (\psi^*\psi)(x)$ is the probability density for finding an electron with wave function $\psi(x)$ at a position $x \in \mathbb{R}^3$. It is a perplexing but characteristic feature of quantum physics that a local description of particle interactions requires the introduction of mathematical objects like gauge potentials $(\phi, \vec{A})$ and complex wave functions ψ that are not directly observable and only certain functions of which can be related to "the real world".[3]

2.1.1 Probability density and probability current density

Born's interpretation of the wave function $\psi(\vec{x}, t)$ implies that the integral over the probability density, i.e. the total probability to find the electron somewhere in space, has to be one:

$$\int d^3x\, \rho(\vec{x}, t) = 1, \qquad \text{with} \qquad \rho(\vec{x}, t) = |\psi(\vec{x}, t)|^2. \tag{2.10}$$

This fixes the normalization of the wave function, which is also called *probability amplitude*, at some initial time up to a phase. Consistency of the interpretation requires that the total probability stays one under time evolution. To check this we compute the time derivative of ρ for a solution of the Schrödinger equation. With $\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A} = \frac{\hbar}{i}(\vec{\nabla} - ig\vec{A})$ for $g = e/(\hbar c)$ and the anti-commutator $\{\vec{\nabla}, \vec{A}\} \equiv \vec{\nabla}\vec{A} + \vec{A}\vec{\nabla} = (\vec{\nabla}\vec{A}) + 2\vec{A}\vec{\nabla}$ we find

$$\begin{aligned}
\dot{\rho}(\vec{x}, t) &= \dot{\psi}^*\psi + \psi^*\dot{\psi} \;=\; (\frac{1}{i\hbar}H\psi)^*\psi + \psi^*\frac{1}{i\hbar}H\psi \\
&= \frac{1}{i\hbar}\frac{\hbar^2}{2m}\Big(\psi(\vec{\nabla} + ig\vec{A})^2\psi^* - \psi^*(\vec{\nabla} - ig\vec{A})^2\psi\Big) \\
&= \frac{\hbar}{2im}\Big(\psi(\Delta + ig\{\vec{\nabla}, \vec{A}\} - g^2\vec{A}^2)\psi^* - \psi^*(\Delta - ig\{\vec{\nabla}, \vec{A}\} - g^2\vec{A}^2)\psi\Big) \\
&= \frac{\hbar}{2im}\Big(\psi\Delta\psi^* - \psi^*\Delta\psi + 2ig\Big((\vec{\nabla}\vec{A})\psi^*\psi + \psi\vec{A}\vec{\nabla}\psi^* + \psi^*\vec{A}\vec{\nabla}\psi\Big)\Big) \\
&= -\vec{\nabla}\left(\frac{\hbar}{2im}(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*) - \frac{e}{mc}\vec{A}\psi^*\psi\right)
\end{aligned} \tag{2.11}$$

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[2] This follows from $(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A}')e^{\frac{ie}{\hbar c}\Lambda} = e^{\frac{ie}{\hbar c}\Lambda}(\frac{\hbar}{i}\vec{\nabla} - \frac{e}{c}\vec{A})$ and $(i\hbar\partial_t - e\phi')e^{\frac{ie}{\hbar c}\Lambda} = e^{\frac{ie}{\hbar c}\Lambda}(i\hbar\partial_t - e\phi)$.

[3] For the electromagnetic potentials this necessity manifests itself in the Aharonov-Bohm effect, which predicts an "action at a distance" of a magnetic field on interference patterns of electrons (see below). This effect was predicted in 1959 and first confirmed experimentally in 1960 [Schwabl].

We thus obtain a continuity equation (similar to the one we know for incompressible fluids)

$$\frac{\partial}{\partial t}\rho(\vec{x},t) + \vec{\nabla}\vec{j}(\vec{x},t) = 0 \tag{2.12}$$

with the *probability current density*

$$\boxed{\vec{j}(\vec{x},t) = \frac{\hbar}{2im}(\psi^*\vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi.) - \frac{e}{mc}\vec{A}\psi^*\psi} \tag{2.13}$$

(It is instructive to compare this formula with the classical particle current $\dot{\vec{x}} = \frac{1}{m}(\vec{p} - \frac{e}{c}\vec{A})$.) By Gauss' theorem, the change in time of the probability to find the particle in a finite volume V equals the flow of the probability current density through the bounding surface ∂V of that domain,

$$\frac{\partial}{\partial t}\int\limits_V \rho(\vec{x},t)d^3x = -\int\limits_V \vec{\nabla}\vec{j}(\vec{x},t)d^3x = -\oint\limits_{\partial V} \vec{j}(\vec{x},t)d\vec{f} \tag{2.14}$$

Normalizability of ψ implies that the fields fall off at infinity so that the surface integral vanishes as $V \to \mathbb{R}^3$. This establishes conservation of the total probability $\int\limits_{\mathbb{R}3} d^3x\,\rho(x) = 1$ for all times.

2.1.2 Axioms of quantum theory

In order to gain some intuition for the physical meaning of the Schrödinger equation we next work out its solutions for a number of simple one-dimensional examples. Before going into the details of the necessary calculations we list here, for later reference, the basic assumptions of quantum mechanics:

1. The state of a quantum system is described by a wave function $\psi(x)$.
2. Observables correspond to self-adjoint operators A (these can be diagonalized and have real eigenvalues).
3. Expectation values of observables (i.e. mean values for repeated measurements of A in the same quantum state) are given by the "scalar product" $\langle A\rangle = \langle\psi|A\psi\rangle = \int \psi^* A\psi$.
4. The time evolution of the system is determined by the Schrödinger equation $i\hbar\frac{\partial\psi}{\partial t} = H\psi$.
5. When the measurement of an observable A yields an eigenvalue a_n then the wave function immediately turns into the corresponding eigenfunction ψ_n of A (this is called collapse of the wave function).

It can be shown that axioms 2 and 3 imply that the result of the measurement of an observable A can only be an eigenvalues a_n of that operator and that the probability for measuring a_n is given by $|c_n|^2$, where c_n is the coefficient of the eigenfunction ψ_n in the expansion $\psi = \sum c_n\psi_n$. In particular, this will imply Born's probability density interpretation of $|\psi(x)|^2$.

2.1.3 Spreading of free wave packets and uncertainty relation

The position and the momentum of a quantum mechanical particle are described by the operators

$$\vec{X}\psi(x) = \vec{x}\psi(x) \qquad \text{and} \qquad \vec{P}\psi(x) = \frac{\hbar}{i}\vec{\nabla}\psi(x), \tag{2.15}$$

respectively. The uncertainty ΔA of a measurement of an observable A in a state ψ is defined as the square root of its mean squared deviation from its expectation value,

$$(\Delta A)^2 = \langle\psi|\,(A - \langle A\rangle_\psi)^2\,|\psi\rangle = \langle A^2\rangle_\psi - (\langle A\rangle_\psi)^2, \tag{2.16}$$

where $\langle A\rangle_\psi = \langle\psi|A|\psi\rangle$ denotes the expectation value of A in the state $\psi(x)$; to be more precise, within the expectation value the number $\langle A\rangle_\psi$ is identified with that number times the unit operator.

For a free particle it can be shown that the uncertainty ΔX of the position increases at late times, i.e. that the wave packets describing localized free particles delocalize and spread out. We now illustrate this phenomenon for a Gaussian wave packet and consider the time evolution of the wave function of a free particle in one dimension, which satisfies the Schrödinger equation with vanishing potential

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) = -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi(x,t). \tag{2.17}$$

Since the Fourier transform $\tilde{\psi}(k)$ of a Gaussian distribution is again a Gaussian we start with a Fourier integral

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}}\int dk\; e^{ikx}\,\tilde{\psi}(k) \tag{2.18}$$

with

$$\tilde{\psi}(k) = \alpha\, e^{-d^2(k-k_0)^2}, \tag{2.19}$$

so that the wave numbers are centered about k_0 with width d. The normalization constant α will be determined later. Since plane waves $e^{i(kx-\omega t)}$ satisfy the free Schrödinger equation if $\omega = \omega(k) = \hbar k^2/(2m)$ we can directly write down the solution for arbitrary times as a Fourier integral

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int dk\;\tilde{\psi}(k)e^{i(kx-\omega t)} = \frac{\alpha}{\sqrt{2\pi}}\int dk\; e^{i(kx-\frac{\hbar k^2}{2m}t)}\; e^{-(k-k_0)^2\,d^2} \tag{2.20}$$

In order to evaluate this integral we bring the exponent into a quadratic form

$$\psi(x,t) = \frac{\alpha}{\sqrt{2\pi}}\int dk \quad e^{-ak^2+2bk-c}, \tag{2.21}$$

where we introduced the combinations

$$a = d^2 + \frac{i\hbar t}{2m}, \qquad b = k_0 d^2 + \frac{ix}{2}, \qquad c = k_0^2 d^2. \tag{2.22}$$

Due to the exponential falloff of the integrand the integration path $-\infty < k < \infty$ can be shifted in the complex plane by the imaginary part of b/a and rotated by the argument of $\sqrt{a}$ without picking up a contribution from the arcs at infinity. Hence we can integrate the new integration variable $\kappa = \sqrt{a}(k - \frac{b}{a})$ again over the real axis and find

$$\psi(x,t) = \frac{\alpha}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\; e^{-a\left(k-\frac{b}{a}\right)^2+\frac{b^2}{a}-c} = \frac{\alpha}{\sqrt{2\pi}}\,e^{\frac{b^2}{a}-c}\int_{-\infty}^{\infty}\frac{d\kappa}{\sqrt{a}}\;e^{-\kappa^2} = \frac{\alpha}{\sqrt{2\pi}}\cdot e^{\frac{b^2}{a}-c}\sqrt{\frac{\pi}{a}}. \tag{2.23}$$

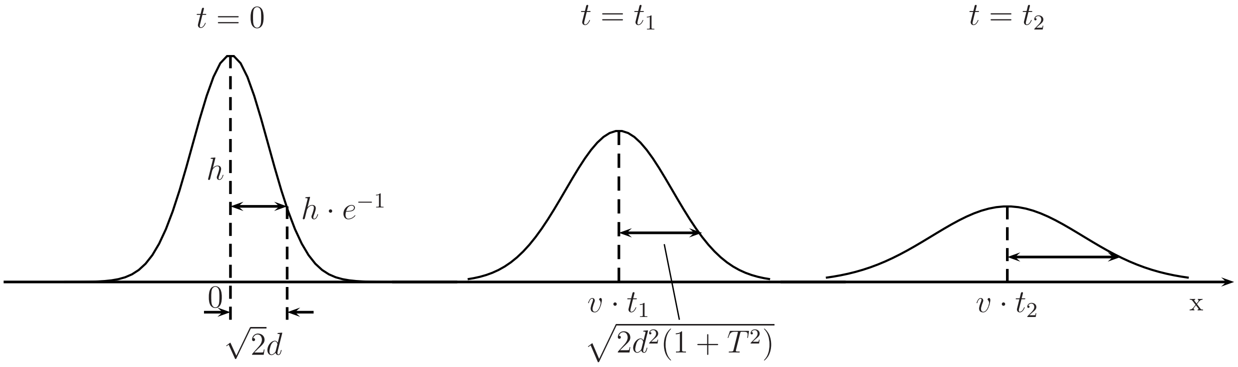

Figure 2.1: Schematic graph of the delocalization of a Gaussian wave packet

For the probability density we obtain

$$|\psi(x,t)|^2 = \frac{|\alpha|^2}{2\pi}\frac{\pi}{|a|} \cdot e^{2Re\left(\frac{b^2-ac}{a}\right)} = \frac{\alpha^2}{2d^2\sqrt{(1+T^2)}} \cdot e^{\frac{-(x-v_0t)^2}{2d^2(1+T^2)}}, \tag{2.24}$$

where we introduced the velocity v_0 and a rescaled time T as

$$\boxed{v_0 = \frac{\hbar k_0}{m}, \qquad\qquad T = \frac{\hbar t}{2md^2}.} \tag{2.25}$$

As expected, the integrated probability density

$$\int dx\ |\psi(x,t)|^2 = \frac{|\alpha|^2}{2d^2\sqrt{(1+T^2)}}\sqrt{2\pi d^2(1+T^2)} = \frac{|\alpha|^2}{d}\sqrt{\frac{\pi}{2}} \tag{2.26}$$

becomes time independent and we find

$$|\alpha|^2 = \sqrt{\frac{2}{\pi}}d. \tag{2.27}$$

$v_0 = \hbar k_0/m$ is the group velocity of the wave packet and for large times $t \gg 2md^2/\hbar$ the width of the wave packet in *position space* becomes proportional to $d\,T = t\hbar/(2md)$ as shown in figure 2.1. Inserting the expressions eq. (2.22) we find the explicit form

$$\psi(x,t) = \frac{\sqrt{1-iT}}{\sqrt{2\pi d(1+T^2)}} \cdot e^{\frac{-(x-v_0t)^2+i(Tx^2+4xk_0d^2-4Tk_0^2d^4)}{4d^2(1+T^2)}} \tag{2.28}$$

for the solution to the Schrödinger equation with initial data $\psi(x,0)$.

Heisenberg's uncertainty relation for position and momentum

In chapter 3 we will derive the general form of Heisenberg's uncertainty relation which, when specialized to position and momentum, reads $\Delta X\,\Delta P \geq \frac{1}{2}\hbar$. Here we check that this inequality is satisfied for our special solution. We first compute the expectation values that enter the uncertainty $\Delta X^2 = \langle (x - \langle x \rangle)^2 \rangle$ of the position.

$$\langle x \rangle = \int x|\psi(x,t)|^2 dx = \int (x - v_0 t)|\psi(x,t)|^2 dx + v_0 t \int |\psi(x,t)|^2 dx = v_0 t. \tag{2.29}$$

The first integral on the r.h.s. is equal zero because the integration domain is symmetric in $x' = x - v_0 t$ and ψ is an even function of x' so that its product with x' is odd. The second integral has been normalized to one. For the uncertainty we find

$$(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle = \int (x - v_0 t)^2 |\psi(x,t)|^2 dx = d^2(1 + T^2), \tag{2.30}$$

where we have used

$$\int_{-\infty}^{+\infty} x^2 e^{-bx^2} dx = -\frac{\partial}{\partial b} \int_{-\infty}^{+\infty} e^{-bx^2} dx = -\frac{\partial}{\partial b}\sqrt{\frac{\pi}{b}} = \sqrt{\frac{\pi}{b}}\frac{1}{2b}, \tag{2.31}$$

i.e. the expectation value of x^2 in a normalized Gaussian integral, as in eq. (2.24), is $\frac{1}{2}$ times the inverse coefficient of $-x^2$ in the exponent.

The uncertainty of the momentum can be computed similarly in terms of the Fourier transform of the wave function since $P = \frac{\hbar}{i}\partial_x = \hbar k$ in the integral representation

$$\int dx\ \psi^* P^n \psi = \int dx \iint \frac{dk\, dk'}{2\pi}\ e^{-i(k'x - \omega' t)} \tilde{\psi}^*(k)(\hbar k)^n e^{i(kx - \omega t)} \tilde{\psi}(k) = \int dk\, |\tilde{\psi}(k)|^2 (\hbar k)^n, \tag{2.32}$$

where $\int dx\, e^{ix(k-k')} = 2\pi\delta(k-k')$ was used to perform the k' integration. Like above, symmetric integration therefore implies $\langle P \rangle = \hbar\langle k \rangle = \hbar k_0$, and by differentiation with respect to the coefficient of $-k^2$ in the exponent of $|\tilde{\psi}(k)|^2$ we find

$$\frac{1}{\hbar^2}(\Delta P)^2 = (\Delta k)^2 = \langle (k - k_0)^2 \rangle = \int (k - k_0)^2 |\tilde{\psi}(k)|^2 = (4d^2)^{-1}. \tag{2.33}$$

The product of the uncertainties is

$$\Delta X \Delta P = \hbar \Delta x \Delta k = \frac{\hbar}{2}\sqrt{1 + T^2} \tag{2.34}$$

which assumes its minimum at the initial time $t = 0$. Hence

$$\boxed{\Delta X \Delta P \geq \frac{\hbar}{2}}. \tag{2.35}$$

Relation (2.35) is known as the *Heisenberg uncertainty relation* and, for this special case, it predicts that one cannot measure position and momentum of a particle at the same time with arbitrary precision. In chapter 3 we will derive the general form of the uncertainty relations for arbitrary pairs of observables and for arbitrary states.

2.2 The time-independent Schrödinger equation

If the Hamiltonian does not explicitly depend on time we can make a separation ansatz

$$\Psi(\vec{x}, t) = u(\vec{x})v(t). \tag{2.36}$$

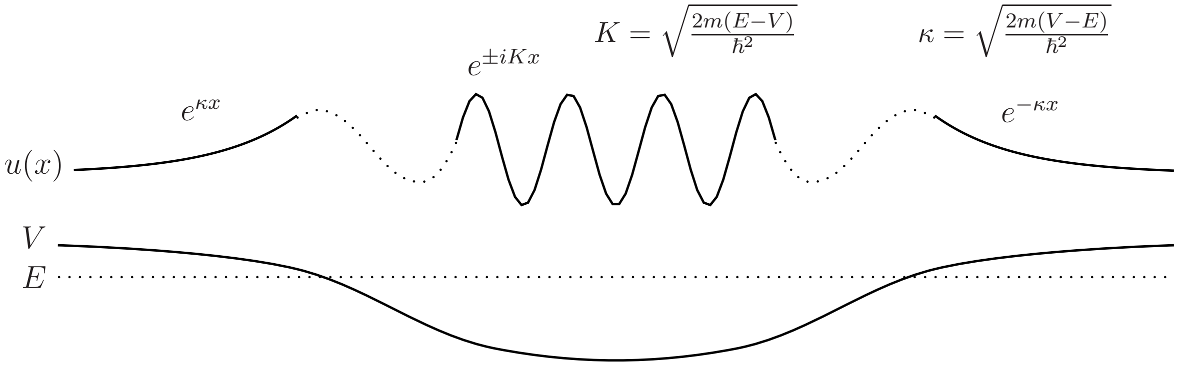

Figure 2.2: Bound state solutions for the stationary Schrödinger equation.

The Schrödinger equation now reads

$$v(t)\left(-\frac{\hbar^2}{2m}\Delta + V(\vec{x})\right)u(\vec{x}) = u(\vec{x})\; i\hbar\frac{\partial}{\partial t}v(t). \tag{2.37}$$

$u(\vec{x})$ and $v(t)$ cannot vanish identically, and except for isolated zeros of these functions we can divide by their product,

$$\frac{1}{u(\vec{x})}\left(-\frac{\hbar^2}{2m}\Delta + V(\vec{x})u(\vec{x})\right) = \frac{1}{v(t)}\left(i\hbar\frac{\partial v(t)}{\partial t}\right) = E. \tag{2.38}$$

The left hand side $(Hu)/u$ depends only on $\vec{x}$ and the right hand side $i\hbar\dot{v}/v$ only on t, therefore both sides of this equation must be equal to a constant E. We thus obtain two separate eigenvalue equations:

$$\left[-\frac{\hbar^2}{2m}\Delta + V(\vec{x})\right]u(\vec{x}) = Eu(\vec{x}) \tag{2.39}$$

and

$$i\hbar\frac{\partial}{\partial t}v(t) = Ev(t). \tag{2.40}$$

Equation (2.39) is known as the *time-independent* or *stationary* Schrödinger equation. Up to constant factor, which is absorbed into a redefinition of $u(x)$, the unique solution to (2.40) is

$$v(t) = e^{-\frac{i}{\hbar}Et} = e^{-i\omega t} \tag{2.41}$$

with the Einstein relation $E = \hbar\omega$. The stationary solutions $\psi(x,t)$ to the Schrödinger equation thus have the form

$$\psi(\vec{x},t) = u(\vec{x})e^{-i\omega t}. \tag{2.42}$$

Their time dependence is a pure phase so that probability densities are time independent.

In order to get an idea of the form of the wave function $u(x)$ we consider a slowly varying and asymptotically constant attractive potential as shown in figure 2.2. Since the stationary Schrödinger equation in one dimension

$$-\frac{\hbar^2}{2m}u''(x) = (E - V(x))\,u(x) \tag{2.43}$$

is a second order differential equation it has two linearly independent solutions, which for a slowly varying $V(x)$ are (locally) approximately exponential functions

$$u(x) \approx \begin{cases} Ae^{iKx} + Be^{-iKx} = A'\sin(Kx) + B'\cos(Kx), & K = \sqrt{\frac{2m(E-V)}{\hbar^2}} \quad \text{for } E > V, \\ Ce^{\kappa x} + De^{-\kappa x} = C'\sinh(\kappa x) + D'\cosh(\kappa x), & \kappa = \sqrt{\frac{2m(V-E)}{\hbar^2}} \quad \text{for } E < V. \end{cases} \tag{2.44}$$

In the classically allowed area, where the energy of the electron is larger then the potential, the solution is oscillatory, whereas in the classically forbidden realm of $E < V(x)$ we find a superposition of exponential growth and of exponential decay. Normalizability of the solution requires that the coefficient C of exponential growth for $x \to \infty$ and the coefficient D of exponential decay for $x \to -\infty$ vanish. If we require normalizability for negative x and increase the energy, then the wave function will oscillate with smaller wavelength in the classically allowed domain, leading to a component of exponential growth of $u(x)$ for $x \to \infty$, until we reach the next energy level for which a normalizable solution exists. We thus find a sequence of wave functions $u_n(x)$ with energy eigenvalues $E_1 < E_2 < \ldots$, where $u_n(x)$ has $n-1$ nodes (zeros). The normalizable eigenfunctions u_n are the wave functions of bound states with a discrete spectrum of energy levels E_n.

It is clear that bound states should exist only for $V_{min} < E < V_{max}$. The lower bound follows because otherwise the wave function is convex, and hence cannot be normalizable. These bounds already hold in classical physics. In quantum mechanics we will see that the energy can be bounded from below even if $V_{min} = -\infty$ (like for the Hydrogen atom). We also observe that *in one dimension* the energy eigenvalues are nondegenerate, i.e. for each E_n any two eigenfunctions are proportional (the vector space of eigenfunctions with eigenvalue E_n is one-dimensional). Normalization of the integrated probability density moreover fixes $u_n(x)$ up to a phase factor (i.e. a complex number ρ with modulus $|\rho| = 1$). Since the differential equation (2.39) has real coefficients, real and imaginary parts of every solution are again solutions. The bound state eigenfunctions $u(x)$ can therefore be chosen to be real.

Parity is the operation that reverses the sign of all space coordinates. If the Hamilton operator is invariant under this operation, i.e. if $H(-\vec{x}) = H(\vec{x})$ and hence the potential is symmetric $V(-\vec{x}) = V(\vec{x})$, then the $u(-\vec{x})$ is an eigenfunction for an eigenvalue E whenever $u(\vec{x})$ has that property because $(H(\vec{x}) - E)u(\vec{x}) = 0$ implies $(H(\vec{x}) - E)u(-\vec{x}) = (H(-\vec{x}) - E)u(-\vec{x}) = 0$. But every function u can be written as the sum of its even part u_+ and its odd part u_-,

$$u(\vec{x}) = u_+(\vec{x}) + u_-(\vec{x}) \qquad \text{with} \qquad u_\pm(\vec{x}) = \frac{1}{2}(u(\vec{x}) \pm u(-\vec{x}) = \pm u_\pm(-\vec{x}). \tag{2.45}$$

Hence $u_\pm$ also solve the stationary Schrödinger equation and all eigenfunctions can be chosen to be either even or odd. In one dimension we know that, in addition, energy eigenvalues are nondegenerate so that u_+ and u_- are proportional, which is only possible if one of these functions vanishes. We conclude that parity symmetry in *one dimension* implies that all eigenfunctions are automatically either even or odd. More precisely, eigenfunctions with an even (odd) number of nodes are even (odd), and, in particular, the ground state u_1 has an even eigenfunction, for the first excited state u_2 is odd with its single node at the origin, and so on.

2.2.1 One-dimensional square potentials and continuity conditions

In the search for stationary solutions we are going to solve equation (2.39) for the simple one-dimensional and time independent potential

$$V(x) = \left\{ \begin{array}{ccc} 0 & \text{for} & |x| \geq a \\ V_0 & \text{for} & |x| < a \end{array} \right. . \tag{2.46}$$

For $V_0 < 0$ we have a potential well (also known as potential pot) with an attractive force and for $V_0 > 0$ a repulsive potential barrier, as shown in figure 2.3. Since the force becomes

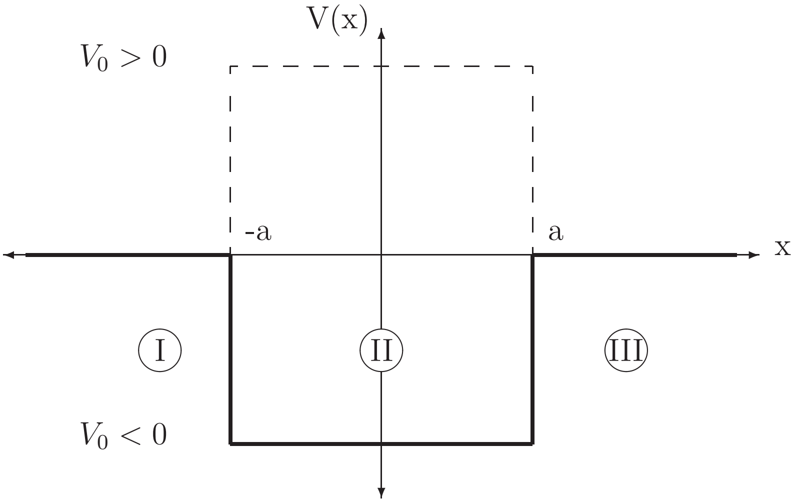

Figure 2.3: One-dimensional square potential well and barrier

infinite (with a δ-function behavior) at a discontinuity of $V(x)$ such potentials are unphysical idealizations, but they are useful for studying general properties of the Schrödinger equation and its solutions by simple and exact calculations.

Continuity conditions

We first need to study the behavior of the wave function at a discontinuity of the potential. Integrating the time-independent Schrödinger equation (2.39) in the form

$$u''(x) = \frac{2m}{\hbar^2}(V - E)u(x) \tag{2.47}$$

over a small interval $[a - \varepsilon, a + \varepsilon]$ about the position a of the jump we obtain

$$\int\limits_{a-\varepsilon}^{a+\varepsilon} u''(x)\, dx = u'(a+\varepsilon) - u'(a-\varepsilon) = \frac{2m}{\hbar^2} \int\limits_{a-\varepsilon}^{a+\varepsilon} (V - E)u(x)\, dx. \tag{2.48}$$

Assuming that $u(x)$ is continuous (or at least bounded) the r.h.s. vanishes for $\varepsilon \to 0$ and we conclude that the first derivative $u'(x)$ is continuous at the jump and only $u''(x)$ has a discontinuity, which according to eq. (2.47) is proportional to $u(a)$ and to the discontinuity of $V(x)$. With $u(a_\pm) = \lim_{\varepsilon\to 0} u(a \pm \varepsilon)$ the matching condition thus becomes

$$u(a_+) = u(a_-) \qquad \text{and} \qquad u'(a_+) = u'(a_-)\,, \tag{2.49}$$

confirming the consistency of our assumption of u being continuous. Even more unrealistic potentials like an infinitely high step for which finiteness of (2.48) requires

$$V(x) = \begin{cases} V_0 & \text{for} \ \ x < a \\ \infty & \text{for} \ \ x > a \end{cases} \qquad \Rightarrow \qquad u(x) = 0 \ \ \text{for } x \ge a\,, \tag{2.50}$$

or δ-function potentials, for which (2.48) implies a discontinuity of u'

$$V(x) = V_{cont.} + A\,\delta(a) \qquad \Rightarrow \qquad \begin{cases} u(a_+) - u(a_-) = 0 \\ u'(a_+) - u'(a_-) = A\,\frac{2m}{\hbar^2}\,u(a) \end{cases}, \tag{2.51}$$

are used for simple and instructive toy models.

2.2.2 Bound states and the potential well

For a bound state in a potential well of the form shown in figure 2.3 we need

$$V_0 < E < 0. \tag{2.52}$$

The stationary Schrödinger equation takes the form

$$\begin{array}{lll} \frac{d^2}{dx^2}u(x) + k^2 u(x) = 0, & k^2 = \frac{2m}{\hbar^2}E = -\kappa^2 & \text{for} \quad |x| > a \\ \frac{d^2}{dx^2}u(x) + K^2 u(x) = 0, & K^2 = \frac{2m}{\hbar^2}(E - V_0) & \text{for} \quad |x| < a \end{array} \tag{2.53}$$

in the different sectors and the respective ansätze for the general solution read

$$\begin{array}{rllll} u_I & = A_1 e^{\kappa x} & + \; B_1 e^{-\kappa x} & for & x \le -a, \\ u_{II} & = A_2 e^{iKx} & + \; B_2 e^{-iKx} & for & |x| < a, \\ u_{III} & = A_3 e^{\kappa x} & + \; B_3 e^{-\kappa x} & for & x \ge a. \end{array} \tag{2.54}$$

For $x \to \pm\infty$ normalizability of the wave function implies $B_1 = A_3 = 0$. Continuity of the wave function and of its derivative at $x = \pm a$ implies the four matching conditions

$$u_I(-a) = u_{II}(-a) \qquad u_{II}(a) = u_{III}(a) \tag{2.55}$$

$$u_I'(-a) = u_{II}'(-a) \qquad u_{II}'(a) = u_{III}'(a) \tag{2.56}$$

or

$$u(-a) = \quad A_1 e^{-\kappa a} = A_2 e^{-iKa} + B_2 e^{iKa}, \qquad u(a) = A_2 e^{iKa} + B_2 e^{-iKa} = B_3 e^{-\kappa a}, \tag{2.57}$$

$$\tfrac{1}{iK}u'(-a) = \tfrac{\kappa}{iK}A_1 e^{-\kappa a} = A_2 e^{-iKa} - B_2 e^{iKa}, \quad \tfrac{1}{iK}u'(a) = A_2 e^{iKa} - B_2 e^{-iKa} = \tfrac{i\kappa}{K}B_3 e^{-\kappa a}. \tag{2.58}$$

These are 4 homogeneous equations for 4 variables, which generically imply that all coefficients vanish $A_1 = A_2 = B_2 = B_3 = 0$. Bound states (i.e. normalizable energy eigenfunctions) therefore only exist if the equations become linearly dependent, i.e. if the determinant of the 4×4 coefficient matrix vanishes. This condition determines the energy eigenvalues because κ and K are functions of the variable E.

Since the potential is parity invariant we can simplify the calculation considerably by using that the eigenfunctions are either even or odd, i.e. $B_2 = \pm A_2$ and $B_3 = \pm A_1$, respectively. With $A_2 = B_2 = \frac{1}{2}A_2'$ for u_{even} and $B_2 = -A_2 = \frac{i}{2}B_2'$ for u_{odd} the simplified ansatz becomes

$$\begin{array}{rcll} u_{even} & = & A_2' \cdot \cos(Kx) & \text{for} \quad 0 < x < a, \\ u_{even} & = & B_3 \cdot e^{-\kappa x} & \text{for} \qquad a < x \end{array} \tag{2.59}$$

and

$$\begin{array}{rcll} u_{odd} & = & B_2' \cdot \sin(Kx) & \text{for} \quad 0 < x < a, \\ u_{odd} & = & B_3 \cdot e^{-\kappa x} & \text{for} \qquad a < x. \end{array} \tag{2.60}$$

In both cases it is sufficient to impose the matching conditions for $x \ge 0$, i.e. at $x = a$. For the even solutions continuity of u and u' implies

$$A_2' \cdot \cos(Ka) \quad = \quad B_3 \cdot e^{-\kappa a} \tag{2.61}$$

$$-KA_2' \cdot \sin(Ka) \quad = \quad -\kappa B_3 \cdot e^{-\kappa a} \tag{2.62}$$

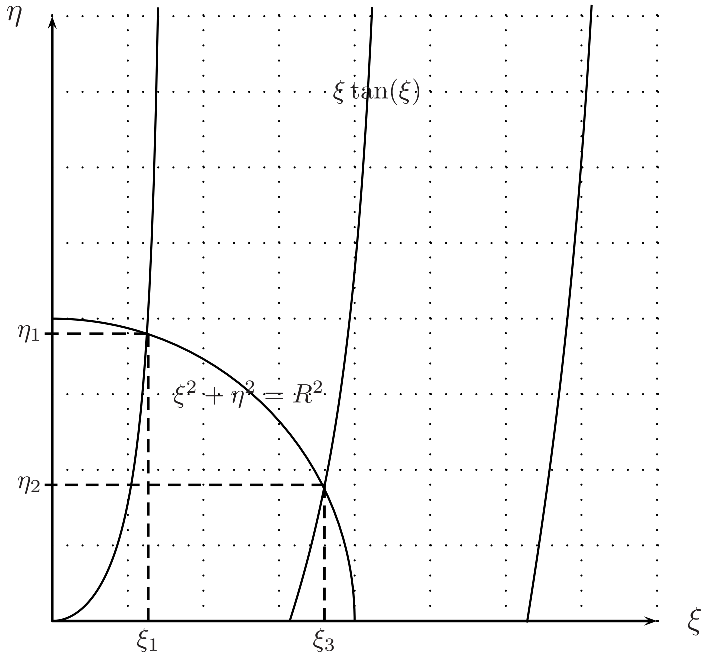

Figure 2.4: Graphical solution of the bound state energy equation for even eigenfunctions.

Taking the quotient we observe that the two equations are linearly dependent if

$$\tan(Ka)=\frac{\kappa}{K}\qquad\text{for }\ u_{even}. \tag{2.63}$$

For the odd case $u(a)=B_2'\sin(Ka)=B_3\cdot e^{-\kappa a}$ and $u'(a)=KB_2'\cos(Ka)=-\kappa B_3\cdot e^{-\kappa a}$ imply

$$\cot(Ka)=-\frac{\kappa}{K}\qquad\text{for }\ u_{odd}. \tag{2.64}$$

The respective wave functions are

$$u(x)=A_1\cdot\begin{cases} e^{\kappa x} & x<-a,\\ e^{-\kappa a}\cdot\frac{\cos(Kx)}{\cos(Ka)} & |x|\le a,\\ e^{-\kappa x} & x>a\end{cases} \tag{2.65}$$

and

$$u(x)=A_1\cdot\begin{cases} e^{\kappa x} & x<-a,\\ e^{-\kappa a}\cdot\frac{\sin(Kx)}{\sin(Ka)} & |x|\le a,\\ -e^{-\kappa x} & x>a\end{cases} \tag{2.66}$$

with $|A_1|$ determined by the normalization integral $\int|u|^2=1$.

The transcendental equations (2.63) and (2.64), which determine the energy levels, cannot be solved explicitly. The key observation that enables a simple graphical solution is that $K^2+\kappa^2=-2mV_0/\hbar^2$ is independent of E. In the (K,κ)–plane the solutions to the above equations therefore correspond to the intersection points of the graphs of these equations with a circle of radius $\sqrt{-2mV_0/\hbar^2}$. It is convenient to set $\xi=Ka$ and $\eta=\kappa a$, hence

$$\eta^2+\xi^2=(\kappa a)^2+(Ka)^2=-\frac{2mE}{\hbar^2}a^2+\frac{2m}{\hbar^2}(E-V_0)a^2=a^2\frac{2m}{\hbar^2}|V_0|=R^2 \tag{2.67}$$

The transcendental equations become

$$\eta = \begin{cases} \xi\tan(\xi) & \text{for } u_{even} \\ -\xi\cot(\xi) & \text{for } u_{odd} \end{cases} \tag{2.68}$$

where only values in the first quadrant $\xi, \eta > 0$ are relevant because K and κ were defined as positive square roots. Figure 2.4 shows the graph of the equations for even wave functions. We observe that there is always at least one solution with $0 < \xi < \pi/2$. The graph of the equation for the odd solutions looks similar with the branches of $-\cot\xi$ shifted by $\pi/2$ as compared to the branches of $\tan\xi$, so that indeed even and odd solutions alternate with increasing energy levels in accord with the *oscillation theorem.* An odd solution only exists if $R > \pi/2$ and for large R the number of bound states is approximately $\frac{2}{\pi}\frac{a}{\hbar}\sqrt{-2mV_0}$. The energy eigenvalues are related by

$$E_n = -\frac{(\hbar\kappa_n)^2}{2m} = -\frac{(\hbar a\eta_n)^2}{2m} = V_0 + \frac{(\hbar a\xi_n)^2}{2m} \tag{2.69}$$

to the common solutions (ξ_n, η_n) of equations (2.67) and (2.68).

2.2.3 Scattering and the tunneling effect

We now turn to the considation of free electrons, i.e. to electrons whose energy exceeds the value of the potential at infinity. In this situation there are no normalizable energy eigenstates and a realistic description would have to work with wave packets that are superpositions of plane waves of different energies. A typical experimental situation is a accelerator where a beam of particles hits an interaction region, with particles scattered into different directions (for the time being we have to ignore the possibility of particle creation or annihilation).

In our one-dimensional situation the particles are either reflected or transmitted by their interaction with a localized potential. If we consider a stationary situation with an infinitely large experminent this means, however, that we do not need a normalizable wave function because the total number of particles involved is infinite, with a certain number coming out of the electron source per unit time. Therefore we can work with a finite and for $x \to \pm\infty$ constant *current density*, which describes the flow or particles. According to the correspondence $p = mv = \frac{\hbar}{i}\partial_x$ we expect that the wave functions

$$u_{right} = Ae^{ikx} \qquad \text{and} \qquad u_{left} = Be^{-ikx} \tag{2.70}$$

describe right-moving and left-moving electron rays with velocities $v = \pm\hbar k/m$, respectively. Indeed, inserting into the formula (2.13) for the probability current density we find

$$j_{right} = \frac{\hbar k}{m}|A|^2 \qquad \text{and} \qquad j_{left} = -\frac{\hbar k}{m}|B|^2. \tag{2.71}$$

As a concrete example we again consider the square potential. For $V_0 > 0$ we have a potential barrier and for $V_0 < 0$ a potential well. Classically all electrons would be transmitted as long as $E > V_0$ and all electrons would be reflected by the potential barrier if $E < V_0$. Quantum mechanically we generically expect to find a combination of reflection and transmission, like in optics. For a high barrier $V_0 > E$ we will find an exponentially suppressed but non-zero probability for electrons to be able to penetrate the classically forbidden region, which is called tunneling effect. Our ansatz for the stationary wave function in the potential of figure 2.5 is

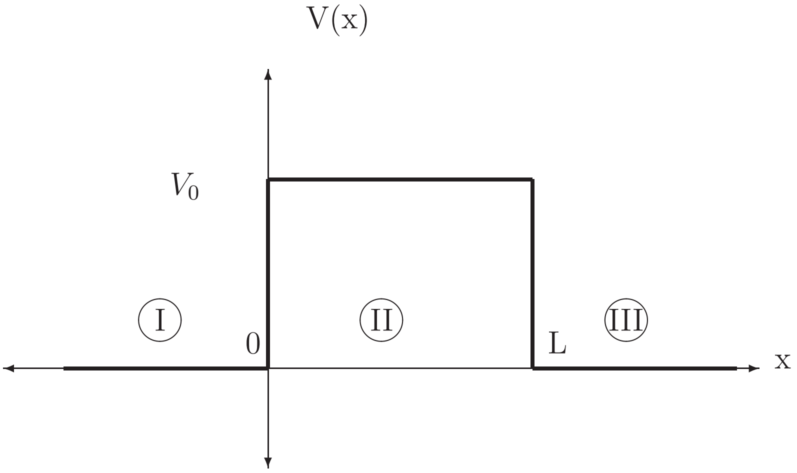

Figure 2.5: Potential barrier

$$u_I = Ae^{ikx} + Be^{-ikx} \qquad \text{for} \qquad x < 0 \qquad \text{with} \qquad k = \sqrt{\tfrac{2mE}{\hbar^2}}, \tag{2.72}$$

$$u_{II} = \begin{cases} Fe^{-\kappa x} + Ge^{+\kappa x} & \text{for} \quad E < V_0 \quad \text{with} \quad \kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}, \\ Fe^{iKx} + Ge^{-iKx} & \text{for} \quad E > V_0 \quad \text{with} \quad K = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} = i\kappa, \end{cases} \tag{2.73}$$

$$u_{III} = Ce^{ikx} + De^{-ikx} \qquad \text{for} \qquad x > L. \tag{2.74}$$

Since for tunneling $E < V_0$ and for the case $E > V_0$ the ansätze in the interaction region II as well as the resulting continuity equations are formally related by $K = i\kappa$, both cases can be treated in a single calculation. Moreover, the ansatz for $E > V_0$ covers scattering at a potential barrier $V_0 > 0$ as well as the scattering at a potential well $V_0 < 0$.

Considering the physical situation of an electron source at $x \ll 0$ and detectors measuring the reflected and the transmitted particles we observe that A is the amplitude for the incoming ray, B is the amplitude for reflection, C is the amplitude for transmission and we have to set $D = 0$ because there is no electron source to the right of the interaction region. We define the two quantities

$$\boxed{\textit{reflection coefficient } R = \left|\frac{j_{ref}}{j_{in}}\right|}, \qquad \boxed{\textit{transmission coefficient } T = \left|\frac{j_{trans}}{j_{in}}\right|}, \tag{2.75}$$

where the *reflection coefficient* R is defined as the ratio of the intensity of the reflected current over the intensity of the incident current and conservation of the total number of electrons implies $T = 1 - R$. Since parity symmetry of the Hamiltonian cannot be used to restrict the *scattering* ansatz to even or odd wave functions, we have shifted the interaction region by $a = L/2$ as compared to figure 2.3. This slightly simplifies some of the intermediate expressions, but of course does not change any of the observables like R and T. Using formulas (2.71) for the currents we find

$$R = \frac{|B|^2}{|A|^2} \qquad \text{and} \qquad T = \frac{|C|^2}{|A|^2}, \tag{2.76}$$

where we used $k_{III}/k_I = v_{III}/v_I = 1$. In situations where the potential of the electron source and the potential of the detector differ the ratio of the velocities has to be taken into account.

For $E > V_0$ continuity of u and u' at $x = 0$,

$$\begin{aligned} A + B &= F + G, \qquad (2.77) \\ ik(A - B) &= iK(F - G), \qquad (2.78) \end{aligned}$$

and at $x = L$,

$$\begin{aligned} Fe^{iKL} + Ge^{-iKL} &= Ce^{ikL}, \qquad (2.79) \\ iK(Fe^{iKL} - Ge^{-iKL}) &= ikCe^{ikL}, \qquad (2.80) \end{aligned}$$

can now be used to eliminate F and G

$$\begin{aligned} 2F = A(1 + \tfrac{k}{K}) + B(1 - \tfrac{k}{K}) &= e^{i(k-K)L}C(1 + \tfrac{k}{K}), \qquad (2.81) \\ 2G = A(1 - \tfrac{k}{K}) + B(1 + \tfrac{k}{K}) &= e^{i(k+K)L}C(1 - \tfrac{k}{K}). \qquad (2.82) \end{aligned}$$

From these equations we can eliminate either C or B,

$$\begin{aligned} e^{2iKL}\Big(A(K^2 - k^2) + B(K - k)^2\Big) &= A(K^2 - k^2) + B(K + k)^2 \qquad (2.83) \\ A\Big((K + k)^2 - (K - k)^2\Big) = 4kKA &= Ce^{ikL}\Big(e^{-iKL}(K + k)^2 - e^{iKL}(K - k)^2\Big) \qquad (2.84) \end{aligned}$$

and solve for the ratios of amplitudes

$$\frac{B}{A} = \frac{(k^2 - K^2)(e^{2iKL} - 1)}{e^{2iKL}(k - K)^2 - (k + K)^2} \qquad (2.85)$$

and

$$\frac{C}{A} = \frac{-4kKe^{-ikL}e^{iKL}}{e^{2iKL}(k - K)^2 - (k + K)^2}. \qquad (2.86)$$

Using $(e^{2iKL} - 1)(e^{-2iKL} - 1) = 2 - e^{2iKL} - e^{-2iKL} = 2(1 - \cos 2Kl) = 4\sin^2 KL$ we determine the reflection coefficient

$$R = \frac{|B|^2}{|A|^2} = \left[1 + \frac{4k^2K^2}{(k^2 - K^2)^2 sin^2(KL)}\right]^{-1} = \left[1 + \frac{4E(E - V_0)}{V_0^2 sin^2(KL)}\right]^{-1} \qquad (2.87)$$

and the transmission coefficient

$$T = \frac{|C|^2}{|A|^2} = \left[1 + \frac{(k^2 - K^2)^2 sin^2(KL)}{4k^2K^2}\right]^{-1} = \left[1 + \frac{V_0^2 sin^2(KL)}{4E(E - V_0)}\right]^{-1}. \qquad (2.88)$$

In general the transmission coefficient T is less than 1, in contrast to classical mechanics, where the particle would always be transmitted. There are two cases with perfect transmission $T = 1$: The first is of course when $V_0 = 0$ and the second is a resonance phenomenon that occurs when $KL = n\pi$ for $n = 1, 2, \ldots$, i.e. when $\sin KL = 0$ so that the length L of the interaction region is a half-integral multiple of the wavelength of the electrons. Conservation of probability $R + T = 1$ holds since $\frac{1}{1+X} + \frac{1}{1+1/X} = 1$.

As we mentioned above the case of a high barrier $V_0 > E$ is related to the formulas for $E > V_0$ by analytic continuation $K = i\kappa$. For the ratios B/A and C/A we hence obtain

$$\frac{B}{A} = \frac{(k^2 + \kappa^2)(e^{2\kappa L} - 1)}{e^{2\kappa L}(k + i\kappa)^2 - (k - i\kappa)^2}, \qquad (2.89)$$

$$\frac{C}{A} = \frac{4ik\kappa e^{-ikL}e^{\kappa L}}{e^{2\kappa L}(k+i\kappa)^2-(k-i\kappa)^2}, \tag{2.90}$$

which leads to the reflection and transmission coefficients

$$R = \frac{|B|^2}{|A|^2} = \left[1+\frac{4k^2\kappa^2}{(k^2+\kappa^2)^2 sinh^2(\kappa L)}\right]^{-1} = \left[1+\frac{4E(V_0-E)}{V_0^2 sinh^2(\kappa L)}\right]^{-1}, \tag{2.91}$$

$$T = \frac{|C|^2}{|A|^2} = \left[1+\frac{(k^2+\kappa^2)^2 sinh^2(\kappa L)}{4k^2\kappa^2}\right]^{-1} = \left[1+\frac{V_0^2 sinh^2(\kappa L)}{4E(V_0-E)}\right]^{-1}. \tag{2.92}$$

For $E < V_0$ neither perfect transmission nor perfect reflection is possible. For large L the transmission probability falls off exponentially

$$T \quad\longrightarrow\quad \frac{16E(V_0-E)}{V_0^2}\, e^{-2\kappa L} \qquad \text{for} \qquad L \gg 1/\kappa. \tag{2.93}$$

The phenomenon that a particle has a positive probability to penetrate a classically forbidden potential barrier is called *tunneling effect*.

2.2.4 Transfer matrix and scattering matrix

The wave functions $u_i(x) = A_i e^{ik_i x} + B_i e^{-ik_i x}$ in domains of constant potential are parametrized by the two amplitudes A_i and B_i. The effect of an interaction region can therefore be regarded as a linear map expressing the amplitudes on one side in terms of the amplitudes on the other side. This map is called *transfer matrix*. For the potential in figure 2.5 and with our ansatz

$$u_I = Ae^{ikx}+Be^{-ikx}, \qquad u_{II} = \begin{cases} Fe^{-\kappa x}+Ge^{+\kappa x} \\ Fe^{iKx}+Ge^{-iKx} \end{cases}, \qquad u_{III} = Ce^{ikx}+De^{-ikx} \tag{2.94}$$

with

$$k=\sqrt{2mE}, \qquad \kappa=\sqrt{2m(V_0-E)}, \qquad K=\sqrt{2m(E-V_0)}=i\kappa \tag{2.95}$$

the matching conditions

$$A+B=F+G \qquad ik(A-B)=iK(F-G) \tag{2.96}$$

can be solved for A and B,

$$\begin{pmatrix} A \\ B \end{pmatrix} = P\begin{pmatrix} F \\ G \end{pmatrix} \qquad \text{with} \qquad P=\frac{1}{2}\begin{pmatrix} 1+\frac{K}{k} & 1-\frac{K}{k} \\ 1-\frac{K}{k} & 1+\frac{K}{k} \end{pmatrix}. \tag{2.97}$$

At $x = L$ we find

$$\begin{pmatrix} F \\ G \end{pmatrix} = Q\begin{pmatrix} C \\ D \end{pmatrix} \qquad \text{with} \qquad Q=\frac{1}{2}\begin{pmatrix} (1+\frac{k}{K})e^{i(k-K)L} & (1-\frac{k}{K})e^{-i(k+K)L} \\ (1-\frac{k}{K})e^{i(k+K)L} & (1+\frac{k}{K})e^{-i(k-K)L} \end{pmatrix}. \tag{2.98}$$

Transfer matrix $M = PQ$ now relates the amplitudes for $x \to \pm\infty$ as

$$\begin{pmatrix} A \\ B \end{pmatrix} = M\begin{pmatrix} C \\ D \end{pmatrix}, \tag{2.99}$$

where A and D are the amplitudes for incoming rays while B and C are the amplitudes for outgoing particles. Because of the causal structure it appears natural to express the outgoing amplitudes in terms of the incoming ones,

$$\begin{pmatrix} B \\ C \end{pmatrix} = S \begin{pmatrix} A \\ D \end{pmatrix}. \tag{2.100}$$

This equation defines the *scattering matrix*, or S-matrix, which can be obtained from the transfer matrix by solving the linear equations $A = M_{11}C + M_{12}D$ and $B = M_{21}C + M_{22}D$ for $B(A, D)$ and $C(A, D)$. We thus find

$$\begin{pmatrix} S_{11} = \frac{M_{21}}{M_{11}} & S_{12} = M_{22} - \frac{M_{12}M_{21}}{M_{11}} \\ S_{21} = \frac{1}{M_{11}} & S_{22} = -\frac{M_{12}}{M_{11}} \end{pmatrix} \tag{2.101}$$

For $D = 0$ we recover the transmission and reflection coefficients as

$$T = \left|\frac{C}{A}\right|^2 = |S_{21}|^2 = \frac{1}{|M_{11}|^2}, \qquad R = \left|\frac{B}{A}\right|^2 = |S_{11}|^2 = \frac{|M_{21}|^2}{|M_{11}|^2} \tag{2.102}$$

(we can think of the index “1´´ as left and of “2” as right; hence $T = S_{21}$ describes scattering from left to right and $R = S_{11}$ describes scattering back to the left).

Conservation of the probability current implies $|B|^2 + |C|^2 = |A|^2 + |D|^2$, i.e. the outgoing current of particles is equal to the incoming current. This can be written as

$$(A^* \ D^*) \begin{pmatrix} A \\ D \end{pmatrix} = |A|^2 + |D|^2 = |B|^2 + |C|^2 = (B^* \ C^*) \begin{pmatrix} B \\ C \end{pmatrix} = (A^* \ D^*)\, S^\dagger\, S \begin{pmatrix} A \\ D \end{pmatrix}, \tag{2.103}$$

where $S^\dagger = (S^*)^T$ is the Hermitian conjugate matrix of S. Since this equality has to hold for arbitrary *complex* numbers A and D we conclude that the S-matrix has to be unitary $S^\dagger S = 1$ or $S^\dagger = S^{-1}$. We thus recover our previous result $R + T = 1$ as the 11-component of the unitarity condition $(S^\dagger S)_{11} = S^*_{11}S_{11} + S^*_{21}S_{21} = 1$.

2.3 The harmonic oscillator

A very important and also interesting potential is the harmonic oscillator potential

$$V(x) = \frac{m\omega_0^2}{2}x^2, \tag{2.104}$$

which is the potential of a particle with mass m which is attracted to a fixed center by a force proportional to the displacement from that center. The harmonic oscillator is therefore the prototype for systems in which there exist small vibrations about a point of stable equilibrium. We will only solve the one-dimensional problem, but the generalization for three dimensions is trivial because $|\vec{x}|^2 = x_1^2 + x_2^2 + x_3^2$ so that $H = H_x + H_y + H_z$. Thus we can make a separation ansatz $u(x, y, z) = u_1(x)u_2(y)u_3(z)$ and solve every equation separately in one dimension. The time independent Schrödinger equation we want to solve is

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega_0^2}{2}x^2\right] u(x) = Eu(x). \tag{2.105}$$

For convenience we introduce the dimensionless variables

$$\xi = \sqrt{\frac{m\omega_0}{\hbar}}\, x, \tag{2.106}$$

$$\lambda = \frac{2E}{\hbar\omega_0}. \tag{2.107}$$

Then the Schrödinger equation reads

$$\left[\frac{\partial^2}{\partial\xi^2} - \xi^2 + \lambda\right] u(\xi) = 0 \tag{2.108}$$

Since $\partial_\xi^2 e^{\pm\frac{1}{2}\xi^2} = (\xi^2 \pm 1)e^{\pm\frac{1}{2}\xi^2}$ the asymptotic behavior of the solution for $\xi \to \pm\infty$ is

$$u(\xi) \backsimeq e^{-\frac{1}{2}\xi^2}, \tag{2.109}$$

where we discarded the case of exponentential growth since we need normalizability. We hence make the ansatz

$$u(\xi) = v(\xi)e^{-\frac{1}{2}\xi^2} \tag{2.110}$$

Inserting into equation (2.108) gives the confluent hypergeometric differential equation:

$$\left[\frac{\partial^2}{\partial\xi^2} - 2\xi\frac{\partial}{\partial\xi} + \lambda - 1\right] v(\xi) = 0 \tag{2.111}$$

This differential equation is often called *Hermite equation* and can be solved by using the power series ansatz

$$v(\xi) = \sum_{\nu=0}^{\infty} a_\nu \xi^\nu. \tag{2.112}$$

The harmonic oscillator potential is symmetric, therefore the eigenfunctions $u(\xi)$ of the Schrödinger equation must have a definite parity. We can therefore consider separately the even and the odd states.

For the even states we have $u(-\xi) = u(\xi)$ and therefore $v(-\xi) = v(\xi)$. So our power series ansatz is

$$v(\xi) = \sum_{\nu=0}^{\infty} a_\nu \xi^{2\nu} \tag{2.113}$$

and contains only *even* powers of ξ. Substituting (2.113) into the the Hermite equation (2.111), we find that

$$\sum_{\nu=0}^{\infty} [2(\nu+1)(2\nu+1)a_{\nu+1} + (\lambda - 1 - 4\nu)a_\nu]\xi^{2\nu} = 0. \tag{2.114}$$

This equation will be satisfied provided the coefficient of each power of ξ separately vanishes, so that we obtain the *recursion relation*

$$a_{\nu+1} = \frac{4\nu + 1 - \lambda}{2(\nu+1)(2\nu+1)} a_\nu. \tag{2.115}$$

Thus, given $a_0 \neq 0$, all the coefficients a_ν can be determined successively by using the above equation. We have therefore obtained a series representation of the even solution (2.113) of the Hermite equation. If this series does not terminate, we see from (2.115) that for large ν

$$\frac{a_{\nu+1}}{a_\nu} \sim \frac{1}{\nu}.$$

This ratio is the same as that of the series for $\xi^{2p} exp(\xi^2)$, where p has a finite value. So we find that the wave function $u(\xi)$ has an asymptotic behavior of the form

$$u(\xi) \sim \xi^{2p} e^{\xi^2/2} \qquad for \;\; |\xi| \to \infty \tag{2.116}$$

which is unacceptable in a physical theory! The only way to avoid this divergence is to require that the series terminates, which means that $v(\xi)$ must be a polynomial in the variable ξ^2. Using the relation (2.115) we see, that the series only terminates, when λ takes on the discrete values

$$\lambda = 4N + 1, \qquad N = 0, 1, 2, ... \;. \tag{2.117}$$

To each value N = 0,1,2,..., of N will then correspond an even function $v(\xi)$ which is a polynomial of order 2N in ξ, and an even, physically acceptable, wave function $u(\xi)$ which is given by (2.113). In a similar way, we obtain the odd states, by using the power series:

$$u(\xi) = \sum_{\nu=0}^{\infty} b_\nu \xi^{2\nu+1} \tag{2.118}$$

which contains only odd powers of ξ. We again substitute the ansatz into the Hermite equation and obtain a recursion relation for the coefficients b_ν. We now see, that the series terminates for the discrete values

$$\lambda = 4N + 3, \qquad N = 0, 1, 2, ... \;.$$

To each value N = 0,1,2,..., of N will then correspond an odd function $v(\xi)$ which is a polynomial of order 2N+1 in ξ, and an odd, physically acceptable wave function $u(\xi)$ given by (2.113). Putting together the results we see that the eigenvalue λ must take on one of the discrete values

$$\lambda = 2n + 1, \qquad n = 0, 1, 2, ... \tag{2.119}$$

where the *quantum number* n is a positive integer or zero. Inserting in (2.107) we therefore find that the energy spectrum of the linear harmonic oscillator is given by

$$\boxed{E_n = \left(n + \frac{1}{2}\right) \hbar\omega_0, \qquad n = 0, 1, 2, ... \;.} \tag{2.120}$$

We see that, in contrast to classical mechanics, the quantum mechanical energy spectrum of the linear harmonic oscillator consists of an infinite sequence of discrete levels! The eigenvalues are *non-degenerate* since for each value of the quantum number n there exists only one eigenfunction (apart from an arbitrary multiplicative constant) and the energy of the lowest state (the *zero-point-energy*) is equal $\hbar\omega/2$, which is clearly non-zero!
Since the wave functions $v_n(\xi)$ are solutions of the Hermite equation and polynomials of the

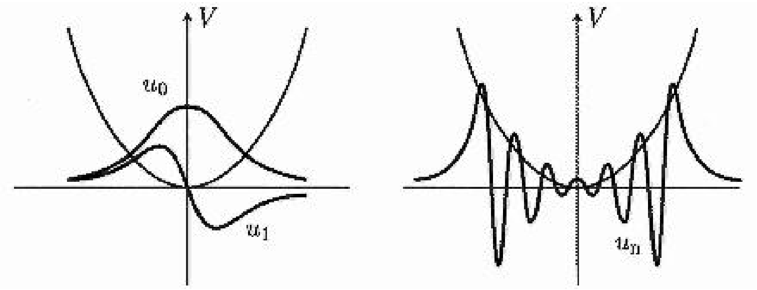

Figure 2.6: Hermite polynomials

order n we will henceforth call them *Hermite polynomials* $H_n(\xi)$. The Hermite polynomials are defined as:

$$\begin{aligned} H_n(\xi) &= (-1)^n e^{\xi^2} \frac{d^n e^{-\xi^2}}{d\xi^n} && (2.121) \\ &= e^{\xi^2/2} \left(\xi - \frac{d}{d\xi} \right)^n e^{-\xi^2/2}, && (2.122) \end{aligned}$$

which leads to the explicit formula

$$H_{2n} = \sum_{k=0}^{n} (-1)^{n-k} \frac{(2n)!(2\xi)^{2k}}{(n-k)!(2k)!}, \qquad H_{2n+1} = 2\xi \sum_{k=0}^{n} (-1)^k \frac{(2n+1)!(2\xi)^{2n-2k}}{k!(2n-2k+1)!} \tag{2.123}$$

for $n \geq 0$. The first few polynomials are

$$\begin{aligned} H_0(\xi) &= 1, && (2.124) \\ H_1(\xi) &= 2\xi, && (2.125) \\ H_2(\xi) &= 4\xi^2 - 2, && (2.126) \\ H_3(\xi) &= 8\xi^3 - 12\xi, && (2.127) \\ H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12, && (2.128) \end{aligned}$$

as shown in figure 2.6.

Another, equivalent, definition of the Hermite polynomials $H_n(\xi)$ involves the use of a *generating function* $G(\xi, s)$:

$$\begin{aligned} G(\xi, s) &= e^{-s^2+2s\xi} \\ &= \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n. && (2.129) \end{aligned}$$

These relations mean that if the function $exp(-s^2 + 2s\xi)$ is expanded in a power series in s, the coefficients of successive powers of s are just $1/n!$ times the Hermite polynomials $H_n(\xi)$. Reinserting the values from the beginning gives to each of the discrete eigenvalues E_n one, and only one, physically acceptable eigenfunction, namely

$$u_n(x) = N_n e^{-\alpha^2 x^2/2} H_n(\alpha x) \qquad where \;\; \alpha = \left(\frac{m\omega}{\hbar} \right)^{1/2}. \tag{2.130}$$

The quantity N_n is a constant which (apart from an arbitrary phase factor) can be determined by requiring that the wave function $u(x)$ be normalized to unity. That is

$$\int |u_n(x)|^2 dx = \frac{|N_n|^2}{\alpha} \int e^{-\xi^2} H_n^2(\xi) d\xi = 1. \tag{2.131}$$

To calculate the normalization constant we use two generating functions of the type (2.129)

$$\begin{aligned} G(\xi, s) &= e^{-s^2+2s\xi} \\ &= \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n. \end{aligned}$$

and

$$\begin{aligned} G(\xi, t) &= e^{-t^2+2t\xi} \\ &= \sum_{m=0}^{\infty} \frac{H_m(\xi)}{m!} t^m. \end{aligned}$$

With these two we may write

$$\int e^{-\xi^2} G(\xi, s) G(\xi, t) d\xi = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{s^n t^m}{n! m!} \int e^{-\xi^2} H_n(\xi) H_m(\xi) d\xi \tag{2.132}$$

Using the fact that

$$\int e^{-x^2} dx = \sqrt{\pi} \tag{2.133}$$

We can calculate the left-hand side of (2.132) to

$$\begin{aligned} \int e^{-\xi^2} e^{-s^2+2s\xi} e^{-t^2+2t\xi} d\xi &= e^{2st} \int e^{-(\xi-s-t)^2} d(\xi - s - t) \\ &= \sqrt{\pi} e^{2st} \\ &= \sqrt{\pi} \sum_{n=0}^{\infty} \frac{(2st)^n}{n!} \end{aligned} \tag{2.134}$$

Equating the coefficients of equal powers of s and t on the right hand sides of (2.129) and (2.134), we find that

$$\int e^{-\xi^2} H_n^2(\xi) d\xi = \sqrt{\pi} 2^n n! \tag{2.135}$$

and

$$\int e^{-\xi^2} H_n(\xi) H_m(\xi) d\xi = 0 \tag{2.136}$$

From (2.131) and (2.135) we see that apart from an arbitrary complex multiplicative factor of modulus one the normalization constant N_n is given by

$$N_n = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2}. \tag{2.137}$$

and hence the normalized linear harmonic oscillator eigenfunctions are given by

$$\boxed{u_n(x) = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} e^{-\alpha^2 x^2/2} H_n(\alpha x).} \tag{2.138}$$

Also these eigenfunctions are orthogonal, so that we can say, the eigenfunctions of the linear harmonic oscillator build a set of orthonormal functions

$$\int u_n^*(x)u_m(x)dx = \delta_{nm}. \tag{2.139}$$

A clear and detailed description of the harmonic oscillator can be found in [Bransden,Joachain].

2.4 Summary

- **The Schrödinger equation :** The Schrödinger equation is the equation of propagation for a wave function $\psi(\vec{x},t)$. It is a homogenous and linear differential equation of the first order with respect to time and second order with respect to space. The general form of the Schrödinger equation is: $H\psi(\vec{x},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t)$ where H is the so called Hamilton operator.

- **Probability current density:** Via time derivation of the probability density $|\psi(\vec{x},t)|^2$ we defined the probability current density $\vec{j}(\vec{x},t) = \frac{\hbar}{2im}(\Psi^*\vec{\nabla}\Psi - (\vec{\nabla}\Psi^*)\Psi)$ which satisfies a continuity equation together with the probability density. With usage of the probability current density we later also defined the
    - Transmission coefficient $T = \left|\frac{j_{trans}}{j_{inc}}\right|$, and the
    - Reflection coefficient $R = \left|\frac{j_{ref}}{j_{inc}}\right|$

- **The free one-dimensional wave packet:** One solution of the free one-dimensional Schrödinger equation is a plane monochromatic wave. In order to be able to normalize and localize the wave/particle we built a wave packet which is a continuous superposition of plane waves. As an example we used a Gaussian wave packet: $\Phi(x,t) = \frac{1}{\sqrt{2\pi}}\int dk e^{i(kx-\frac{\hbar k^2}{2m}t)}\alpha\cdot e^{-(k-k_0)^2\cdot d^2}$ In the following calculations we discovered, that the wave packet "delocalizes" with time.

- **The Heisenberg uncertainty relation:** As a direct result of the solution of the free one-dimensional Schrödinger equation we found that the product of position uncertainty and momentum uncertainty is given by: $\Delta x\Delta p \geq \frac{\hbar}{2}$ where the uncertainties follow the definition $(\Delta A)^2 = \langle(A - \langle A\rangle)^2\rangle$ and $\langle A\rangle$ is the mean value of a.

- **The potential well:** For the negative potential $-V_0$ we differentiated two cases: $V_0 < E < 0$, so called boundary states, and $E > 0$, so called scattering states. Solving the Schrödinger equation for the boundary states and using the continuity conditions led to discrete Energy eigenvalues and eigenstates. In case of scattering states we introduced the reflection coefficient and the transmission coefficient. Calculating these we came to the interesting result that unlike classical mechanics a particle has a certain probability to be reflected from the well, even if its energy is greater than zero!

- **The potential barrier:** Again we differentiated two cases (now for the potential $V_0 > 0$): $0 \leq E \leq V_0$ and $V_0 < E$. In both cases we calculated R and T. We came to the result, that like for the potential well there is a certain probability for the particle to be reflected even if $V_0 < E$ and most stunning there is a probability for the particle to be transmitted even for $0 \leq E \leq V_0$. The latter we call *tunnel effect*.

- **The harmonic oscillator:** We solved the Schrödinger equation for the harmonic oscillator potential $V(x) = \frac{m\omega_0^2}{2}x^2$. The calculation resulted in a discrete spectrum of energy eigenvalues: $E_n = \left(n + \frac{1}{2}\right)\hbar\omega_0, \quad n = 0, 1, 2, ...$ and to each eigenvalue an eigenfunction $u_n(x) = \left(\frac{\alpha}{\sqrt{\pi}2^n n!}\right)^{1/2} e^{-\alpha^2 x^2/2} H_n(\alpha x)$. An interesting fact is that the zero-point-energy is $\hbar\omega/2$ and thus non zero!

- **Further reading:** For more detailed information on wave mechanics and the Schrödinger equation we suggest [Bransden,Joachain] and [Messiah]. Also for a very intuitive explanation of the uncertainty principle we recommend [Feynman], volume 3, chapter one.